**Annotated Bibliography**
**Applied Physics Review Paper**
**Nathan S Johnson et al.**

To be organized alphabetically by citation key.


- Mostafa Abdelrahman, Edward W. Reutzel amd Abdalla R. Nassar, and Thomas L. Starr. Flaw detection in powder bed fusion using optical imaging. *Additive Manufacturing*, 15:1–11, February 2017 **Details a computer vision approach to detecting flaws during builds of LPBF.**
  - **Computer vision**
  - **In situ monitoring**
- Noga Alon, Shai Ben-David, Nicolo Cesa-Bianchi, and David Haussler. Scale-Sensitive Dimensions, Uniform Convergence, and Learnability. *Journal of the ACM*, 44(4):615–631, 1997 **Details the conditions necessary for success in some classes of learners; specifically details conditions necessary on Glivenko-Cantelli classes.**
- A.A. Antonysamy, J. Meyer, and P.B. Prangell. Effect of build geometry on the $\beta$-grain structure and texture in additive manufacture of ti-6al-4v by selective electron beam melting. *Materials Characterization*, 84:153–168, October 2013 **Study of grain structure and texture in powder bed e-beam Ti-6Al-4V; observes prior beta grain grown aligned in $\langle 0001 \rangle$ normal to build direction; contour layer has different grain structure.**
  - **Parametric analysis – build geometry (angle, wall thickness, geometry, etc.) $\rightarrow$ grain structure**
- S.H. Mousavi Anijdan, A. Bahrami, H.R. Madaah Hosseini, and A. Shafyei. Using genetic algorithm and artificial neural network analyses to design an al-si casting alloy of minimum porosity. *Materials and Design*, 27:605–609, 2006 **Used an ANN and GA to correlate chemical composition and cooling rate to porosity in Al-Si.**
  - **Alloy Design**
- Christopher J. Bartel, Samantha L. Millican, Ann M. Deml, John R. Rumptz, William Tumas, Alan W. Weimer, Stephan Lany, Valadan Stevanović, Charles B. Musgrave, and Aaron M. Holder. Physical descriptor for the gibbs energy of inorganic crystalline solids and temperature dependent materials chemistry. *Nature Communications*, 9(4168), 2018 **Uses SISSO to generate a descriptor which can predict Gibbs free energy from entries in the ICSD**
- Bernd Baufeld, Erhard Brandl, and Omer Van Der Biest. Wire based additive layer manufacturing: Comparison of microstructure and mechanical properties of Ti-6Al-4V components fabricated by laser-beam deposition and shaped metal deposition. *Journal of Materials Processing Technology*, 211(6):1146–1158, 2011 **Compares microstructure and mechanical properties of Ti-6Al-4V fabricated by shaped metal deposition versus additive layer manufacturing (wire-based AM)**
  - **Parametric analysis – manufacturing process (SMD vs laser DED) $\rightarrow$ microstructure**
- Herbert Bay, Andreas Ess, Tinne Tuytelaars, and Luc Van Gool. Speeded-up robust features. *Computer Vision and Image Understanding*, 110:346–359, 2008 **Citation of original paper for speeded-up robust feature (SURF) algorithm.**
  - **Computer vision**
- Jörg Behler. Constructing high-dimensional neural network potentials: A tutorial review. *International Journal of Quantum Chemistry*, 115(16):1032–1050, 2015 **Details theoretical development of atomic potentials using neural networks; method of model approximation using machine learning (instead of DFT).**
- Umberto Scipioni Bertoli, Gabe Guss, Sheldon Wu, Manyalibo J. Matthews, and Julie M. Schoenung. In-situ characterization of laser-power interaction and cooling through high-speed imaging of powder bed fusion additive manufacturing. *Materials and Design*, 135:385–396, 2017 **Study using high speed imaging to monitor melt pools in SLM; experimentally determines cooling rates.**

– **In sit monitoring**


- Sebastian Berumen, Florian Bechmann, Stefan Lindner, Jean-Pierre Kruth, and Tom Craeghs. Quality control of laser- and powder bed-based Additive Manufacturing (AM) technologies. *Physics Procedia*, 5:617–622, 2010 **Uses basic detection techniques to study and monitor melt pool in SLM; has good explanation of physics of melt pools.**

  – **In situ monitoring**

- M. A. Bessa, R. Bostanabad, Z. Liu, A. Hu, Daniel W. Apley, C. Brinson, W. Chen, and Wing Kam Liu. A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality. *Computer Methods in Applied Mechanics and Engineering*, 320:633–667, 2017 **Framework for design and modeling of new material systems – framework is as follows: 1. design of experiments, optimizing on microstructure, phase properties, and 'external conditions,' 2. computational analyses based on sample design, generate material response database, 3. machine learning to database of generated materials**

- Jack Beuth and Nathan Klingbeil. The role of process variables in laser-based direct metal solid freeform fabrication. *Journal of Materials: Laser Processing*, September 2001 **Outlines the creation of process maps for predicting melt pool size, thermal gradients, maximum residual stresses, and more.**

- H. K. D. H. Bhadeshia, R. C. Dimitriu, S. Forsik, J. H. Pak, and J. H. Ryu. Performance of neural networks in materials science. *Materials Science and Technology*, 25(4):504–510, 2009 **Addresses the use of neural networks in materials science; presents a loose guideline for maximising the impact of neural network models created.**

- G. Bi, C. N. Sun, and A. Gasser. Study on influential factors for process monitoring and control in laser aided additive manufacturing. *Journal of Materials Processing Technology*, 213(3):463–468, 2013 **Study on process monitoring in laser aided additive manufacturing; looks at powder density, beam focus, defect generation, oxidation, dimensional accuracy.**

  – **Alloy Design**

- C.D. Boley, S.C. Mitchell, A.M. Rubenchik, and S.S.Q. Qu. Metal powder absorptivity: modeling and experiment. *Applied Optics*, 55(23):6496–2501, August 2016 **Research article from LLNL on absorptivity measurements of metal powders; has applications to simulation of LPBF process.**

  – **Alloy design**

- Srikanth Bontha, Nathan W. Klingbeil, Pamela A. Kobryn, and Hamish L. Fraser. Thermal process maps for predicting solidification microstructure in laser fabrication of thin-wall structures. *Journal of Materials Processing Technology*, 178:135–142, March 2006 **Develops thermal process maps relating cooling rate and thermal gradient to laser power and velocity; looking at a LENS process; uses 2D rosenthal solution for the melt pool depth; compares with 2D nonlinear thermal finite element model**

  – **Parametric analysis – laser power & velocity → cooling rate temperature gradient**

- Srikanth Bontha, Nathan W Klingbeil, Pamela A Kobryn, and Hamish L Fraser. Effects of process variables and size scale on solidification microstructure in beam-based fabrication of bulk 3d structures. *Materials Science and Engineering A*, 513-514:311–318, 2009 **Study of size effects on microstructure formation in electron beam on a generalized additive process; investigations heat transfer using a 3D rosentathal solution for a moving point source; develops thermal process maps to predict microstructure type (columnar versus equiaxed).**

  – **Parametric analysis – cooling rate and temperature gradient → grain morphology**

- Leo Breiman. Some properties of splitting criteria. *Machine Learning*, 24:41–47, 1996 **Citation of an original paper on random forests.**

- Leo Breiman. Random forests. *Machine Learning*, 45(1):5–32, 2001 **Another citation of a paper on random forests.**

- Craig A. Brice, Wesley A. Tayon, John A. Newman, Milo V. Kral, Catherine Bishop, and Anna Sokolova. Effect of compositional changes on microstructure in additively manufactured aluminum alloy 2139. *Materials Characterization*, April 2018 **A design of experiments study whereby nine different experiments were conducted on an aluminum alloy to determine impact of composition, substrate temperature on magnesium loss; found that changes in Mg content can impact microstructure significantly.**
  - **Design of experiments**
  - **Parametric analysis – composition, substrate heating → microstructure**
- Rasmus Bro and Age K. Smilde. Principal component analysis. *Analytical Methods Tutorial Review*, 6(2812), 2014 **Overview of PCA methods.**
  - **Dimensionality reduction via matrix factorization review**
- Keith T. Butler, Daniel W. Davies, Hugh Cartwright, Olexandr Isayev, and Aron Walsh. Machine learning for molecular and materials science. *Nature Reviews*, 559, July 2018 **A review article on applications of machine learning in molecular and materials sciences; outlines machine learning techniques that are suitable for certain research questions.**
- J. Carrete, W. Li, N. Mingo, S. Wang, and S. Curtarolo. Finding Unprecedentedly low-thermal-conductivity half-Heusler semiconductors via high-throughput materials modeling. *Phys. Rev. X*, 4(1):011019, 2014 **Example of the success of random forests in predicting material behavior.**
- G Ceder, Y.-M. Chiang, D R Sadoway, M K Aydinol, Y.-I. Jang, and B Huang. Identification of cathode materials for lithium batteries guided by first-principles calculations. *Nature*, 392(6677):694–696, 1998 **An early example of how ab initio searches can be used for discovery of compounds with certain properties**
- N. Chakraborti. Genetic algorithms in materials design and processing. *International Materials Reviews*, 49(3-4):246–272, 2004 **Review of genetic algorithms in materials design; divided into three main sections: review of genetic algorithms, genetic algorithms in materials design, genetic algorithms in materials processing.**
- Long-Qing Chen. Phase-field models for microstructure evolution. *Annual Review of Materials Research*, 32:113–140, 2002 **Describes phase field modeling for modeling microstructure evolution at the mesoscale.**
  - **Phase field model**
  - **ICME**
- Hailong Chen, Geoffroy Hautier, Anubhav Jain, Charles Moore, Byoungwoo Kang, Robert Doe, Lijun Wu, Yimei Zhu, Yuanzhi Tang, and Gerbrand Ceder. Carbonophosphates: A new family of cathode materials for Li-ion batteries identified computationally. *Chemistry of Materials*, 24(11):2009–2016, 2012 **New class of Li-ion battery cathode materials discovered through high throughput ab initio searches.**
- Yuan Chen, Fenggui Lu, Ke Zhang, Pulin Nie, Seyed Reza Elmi Hosseini, Kai Feng, and Zhuguo Li. Dendritic microstructure and hot cracking of laser additive manufactured inconel 718 under improved base cooling. *Journal of Alloys and Compounds*, 670:312–321, October 2016 **Observation of texture, microstructural characteristics of SLM Inconel 718; studies orientation of dendritic grains as a function of base temperature; looks are cracking in heat affected zone.**
  - **Parametric analysis – substrate/base cooling temperature → hot cracking behavior**
- R.P. Cherian, L.N. Smith, and P.S. Midha. A neural network approach for selection of powder metallurgy materials and process parameters. *Artificial Intelligence in Engineering*, 14(1):39–44, 2000 **Covers use of a neural network to predict mechanical properties from parts formed using powder metallurgy.**
- J.A. Cherry, H. M Davies, S. Mehmood, N. P. Lavery, S. G. R. Brown, and J. Sienz. Investigation into the effect of process parameters on microstructural and physical properties of 316l stainless steel parts by selective laser melting. *International Journal of Advanced Manufacturing Technology*, 76:869–879, September 2015 **Study on SLM of 316L SS; investigated impact of process parameters on surface roughness, porosity, and hardness.**

  - **Parametric analysis – laser energy density → surface finish, microstructure, density, hardness**
  - **More specifics: they varied laser energy density by varying exposure time and point distance (amount of overlap between hatches)**

- Aritra Chowdhury, Elizabeth Kautz, Bülent Yener, and Daniel Lewis. Image driven machine learning methods for microstructure recognition. *Computational Materials Science*, 123:176–187, 2016 **Applied computer vision and machine learning to automate recognition of microstructural features; visual bag of words, texture, pre-trained convolutional neural network used for feature extraction; classified dendritic versus non dendritic using support vector machine, voting, nearest neighbor, and random forests.**
  - **In situ monitoring**
  - **Computer vision**
- Cristian V. Ciobanu, Dhananjay T. Tambe, and Vivek B. Shenoy. First-principles calculations of step formation energies and step interactions on tin(0 0 1). *Surface Science*, 582:145–150, 2005 **A citation for Ciobanu that Stebner asked for.**
- P.C. Collins, D.A. Brice, P. Samimi, I. Ghamarian, and H.L. Fraser. Microstructure control of additively manufactured metallic materials. *Annual Review of Materials Research*, 46:63–91, May 2016 **Attempts to establish a framework that incorporates processing variables, alloy composition, and thee resulting microstructure.**
- Stefano Curtarolo, Dane Morgan, Kristin Persson, John Rodgers, and Gerbrand Ceder. Predicting Crystal Structures with Data Mining of Quantum Calculations. *Physical Review Letters*, 91(13):135503, 2003 **Uses principal component analysis on ab initio energy calculations to study correlations in crystal structure and formation energy.**
  - **Dimensionality reduction**
  - **Matrix factorization**
- Stefano Curtarolo, Dane Morgan, and Gerbrand Ceder. Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, 29(3):163–211, 2005 **A study on the accuracy of ab initio methods.**
- Stefano Curtarolo, Wahyu Setyawan, Gus L W Hart, Michal Jahnatek, Roman V. Chepulskii, Richard H. Taylor, Shidong Wang, Junkai Xue, Kesong Yang, Ohad Levy, Michael J. Mehl, Harold T. Stokes, Denis O. Demchenko, and Dane Morgan. AFLOW: An automatic framework for high-throughput materials discovery. *Computational Materials Science*, 58:218–226, 2012 **Introduces AFLOW.**
- Stefano Curtarolo, Wahyu Setyawan, Shidong Wang, Junkai Xue, Kesong Yang, Richard H. Taylor, Lance J. Nelson, Gus L W Hart, Stefano Sanvito, Marco Buongiorno-Nardelli, Natalio Mingo, and Ohad Levy. AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. *Computational Materials Science*, 58:227–235, 2012 **Introduces AFLOWLIB.**
- Stefano Curtarolo, Gus L. W. Hart, Marco Buongiorno Nardelli, Natalio Mingo, Stefano Sanvito, and Ohad Levy. The high-throughput highway to computational materials design. *Nature Materials*, 12(3):191–201, 2013 **A review of high throughput ab initio methods in DFT and how they can be beneficial to materials design.**
- Donghua Dai and Dongdong Gu. Thermal behavior and densification mechanism during selective laser melting of copper matrix composites: Simulation and experiments. *Materials and Design*, 55:482–491, October 2014 **Simulation of temperature profile and densification of SLM using a finite volume method; models transition from powder to solid as well as surface tension induced by temperature gradient; studies impact of power; shows asymmetric temperature distribution wrt laser scanning area.**
  - **Finite element thermomechanical model**
  - **ICME model**
- D. M. Deaven and K. M. Ho. Molecular geometry optimization with a genetic algorithm. *Physical Review Letters*, 75(2):288–291, 1995 **Describes a method of optimizing the charge balance between atoms based on position using a genetic algorithm approach. Pretty cool paper if you ask me.**

- Brian L. Decost and Elizabeth A. Holm. A computer vision approach for automated analysis and classification of microstructural image data. *Computational Materials Science*, 110:126–133, 2015 **Uses bag of visual features to create synthetic microstructural images; classifies generated images using a support vector machine.**
  - **Computer vision**
- Brian L. DeCost, Harshvardhan Jain, Anthony D. Rollett, and Elizabeth A. Holm. Computer Vision and Machine Learning for Autonomous Characterization of AM Powder Feedstocks. *Jom*, 69(3):456–465, 2017 **Characterizes powder feedstock materials; uses SIFT for feature extraction; classifies powder particles.**
  - **Computer vision**
- Brian L. DeCost and Elizabeth A. Holm. Characterizing powder materials using keypoint-based computer vision methods. *Computational Materials Science*, 126:438–445, 2017 **Applies bag of visual words to classify images of powder particles based on particle size distribution, morphology, and surface texture.**
  - **Computer vision**
- Brian L. DeCost, Toby Francis, and Elizabeth A. Holm. Exploring the microstructure manifold: image texture representations applied to ultrahigh carbon steel microstructures. *Acta Materialia*, 133:30–40, 2017 **Uses t-SNE to graphically explore datasets of microstructures at a range of scales in Ultrahigh carbon steel; ultrahigh carbon steel is known for having complex, hierarchical structures.**
  - **Dimensionality reduction**
- R. R. Dehoff, M. M. Kirka, W. J. Sames, H. Bilheux, A. S. Tremsin, L. E. Lowe, and S. S. Babu. Site specific control of crystallographic grain orientation through electron beam additive manufacturing. *Materials Science and Technology*, 31(8), October 2015 **Title kind of says it all; uses careful control of thermal gradient (G) and solidification velocity (R) in order to control crystallographic growth direction if Inconel 718; uses neutron diffraction to characterize texture.**
- Maarten de Jong, Wei Chen, Henry Geerlings, Mark Asta, and Kristin Aslaug Persson. A database to enable discovery and design of piezoelectric materials. *Scientific Data*, 2:150053, 2015 **Introduces a database for discovery of piezoelectric materials.**
- Jordi Delgado, Joaquim Ciurana, and Ciro A. Rodriguez. Influences of process parameters on part quality and mechanical properties for dmls and slm with iron-based materials. *International Journal of Advanced Manufacturing Technology*, 60:601–610, September 2012 **Full-factorial design of experiments for investigating manufacturing parameters on macroscopic mechanical properties; an 'early' paper investigating impact of processing parameters on quality**
  - **Design of Experiments**
  - **Parametric analysis – scan speed, layer thickness, build orientation → distortion, surface roughness, mechanical properties**
- Zhenghua Deng, Haiqing Yin, Xue Jiang, Cong Zhang, Kaiqi Zhang, Tong Zhang, Bin Xu, Qingjun Zheng, and Xuanhui Qu. Machine learning aided study of sintered density in cu-al alloy. *Computational Materials Science*, 155:48–54, July 2018 **Picks certain descriptors to predict sintered density of Cu-Al alloy using multilayer perceptron, neural networks; descriptors were chosen from processing parameters, composition, property of raw materials.**
- Erik R. Denlinger, Jarred C. Heigel, Pan Michaleris, and T.A. Palmer. Effect of inter-lay dwell time on distortion and residual stress in additive manufacturing of titanium and nickel alloys. *Journal of Materials Processing Technology*, 215:123–131, August 2015 **In situ measurements of part distortion are made for titanium and nickel alloys as a function of dwell time between deposition of material; laser based powder bed study; also studied residual stress build up as a function of dwell time.**
  - **Parametric analysis – laser dwell time → part distortion from residual stresses**
  - **In situ**

- Juan J. De Pablo, Barbara Jones, Cora Lind Kovacs, Vidvuds Ozolins, and Arthur P. Ramirez. The Materials Genome Initiative, the interplay of experiment, theory and computation. *Current Opinion in Solid State and Materials Science*, 18(2):99–117, 2014 **This article is from an NSF workshop in 2014 on the MGI; it details areas of recent growth, areas of need, central challenges related to, and perspectives on materials informatics, under the umbrella of the 'Materials Genome Initiative'; focuses mainly on modeling.**

- J. Ding, P. Colegrove, J. Mehnen, S. Ganguly, P.M. Sequeira Almeida, F. Wang, and S. Williams. Thermo-mechanical analysis of wire and arc additive layer manufacturing process on large multi-layer parts. *Computational Materials Science*, 50:3315–3322, July 2011 **Large scale (>500mm) finite element model of gas WAAM; focused on residual stress development and temperature history; generated temperature vs time and location for single-wall builds; also simulated distortion**
  - **Large scale model**
  - **Finite element residual stress**
  - **ICME model**

- S.V. Dudiy and Alex Zunger. Searching for alloy configurations with target physical properties: Impurity design via a genetic algorithm inverse band structure approach. *Physical Review Letters*, 97, July 2006 **Study on using genetic algorithms to design a material with a specific band gap; inverse band gap design; good explanation of genetic algorithms using natural language; great paper for alloy design.**
  - **Alloy Design**

- Bradley Efron. Estimation and accuracy after model selection. *Journal of the American Statistical Association*, 109(507):991–1007, 2014 **A text on bootstrap methods of estimating standard errors with consideration of model selection.**

- Christopher C. Fischer, Kevin J. Tibbetts, Dane Morgan, and Gerbrand Ceder. Predicting crystal structure by merging data mining with quantum mechanics. *Nature Materials*, 5(8):641–646, 2006 **They essentially develop their own data mining approach to predict the probability of a given composition forming a certain stable crystal structure.**
  - **Alloy Design**

- José A. Flores-Livas, Antonio Sanna, and Stefan Goedecker. Accelerated materials design approaches based on structural classification: application to low enthalpy high pressure phases of SH3 and SeH3. *Novel Superconducting Materials*, 3(1):6–13, 2017 **I am not sure how I found this article; study on using a unique representation of crystal structures as part of a search algorithm; searches for stable crystal structures as a function of pressure; has a good lit review on machine learning methods for crystal structure prediction.**

- Ian Foster, Rachana Ananthakrisnan, Ben Blaiszik, Kyle Chard, Ray Osborn, Steven Tuecke, Mike Wilde, and Justin Wozniak. Networking materials data: Accelerating discovery at an experimental facility. *Big Data and HPC*, 2015 **Discusses HPC methods for the types of analysis that go on at Argonne National Laboratory.**

- Alberto Fransceschetti and Alex Zunger. The inverse band-structure problem of finding an atomic configuration with given electronic properties. *Letters to Nature*, 402, November 1999 **They describe an algorithmic approach to predicting the crystal structure of various compositions grown using molecular beam epitaxy or metallographic chemical vapor deposition; high-throughput study.**
  - **Alloy Design**

- M.M. Francois, A. Sun, W.E. King, N.J. Henson, D. Tourret, C.A. Bronkhorst, N.N. Carlson, C.K. Newman, T. Haut, J. Bakosi, J.W. Gibbs, V. Livescu, S.A. Vander Wiel, A.J. Clarke, M.W. Schraad, T. Blacker, H. Lim, T. Rodgers, S. Owen, F. Abdeljawad, J. Madison, A.T. Anderson, J-L. Fattebert, R.M. Ferencz, N.E. Hodge, S.A. Khairallah, and O. Walton. Modeling of additive manufacturing processes for metals: Challenges and opportunities. *Current Opinion in Solid State and Materials Science*, pages 1–9, 2017 **This is a review of modeling methods and challenges in wire feed and powder bed AM; covers a range of scales from microscale to macroscale; compiled by the three major DOE labs.**

  - **ICME Review**

- William E. Frazier. Metal additive manufacturing: A review. *Journal of Materials Engineering and Performance*, 23(6):1917–1928, 2014 **Big ass, low level review of additive manufacturing; covers all the processes you would ever need.**

- Wei Gao, Yunbo Zhang, Devarajan Ramanujan, Karthik Ramani, Yong Chen, Christopher B Williams, Charlie. C L Wang, Yung C Shin, Song Zhang, and Pablo D Zavattieri. The status, challenges, and future of additive manufacturing in engineering. *Computer-Aided Design*, 69:65–89, 2015 **Review of state of the art for AM and challenges for AM; reviews all 3D printing applications, not just metal; goes into the process of how a CAD file is used to create a 3D printed part; discusses societal and logistical impacts.**

- Leon A. Gatys, Alexander S. Ecker, and Matthias Bethge. Texture Synthesis Using Convolutional Neural Networks. pages 1–10, 2015 **Generates a database of synthetic textures for use with image recognition in human brains; more focused on neuroscience.**

- M.W. Gaultois, A.O. Oliynyk, A. Mar, T.D. Sparks, G.J. Mulholland, and B. Meredig. Perspective: Web-based machine learning models for real-time screening of thermoelectric materials properties. *APL Materials*, 4(5):053213, 2016 **Case study of Citrine's web-based random forest platform on a database of thermoelectric materials.**

  - **Model reduction**

- Andrew T. Gaynor and James K. Guest. Topology optimization considering overhang constraints: Elimination sacrificial support material in additive manufacturing through design. *Structural and Multidisciplinary Optimization*, 54:1157–1172, September 2016 **Topology optimization specifically to reduce the amount of sacrificial support structures that need to be used.**

  - **Topology optimization**

- Ghiringhelli Kyca N, Jan Vybiral, Sergey V. Levechenko, Claudia Draxl, and Matthias Scheffler. Big data of materials science - critical role of the descriptor. *arXiv*, February 2015 **A great paper; discusses finding improved descriptors for predicting material properties.**

- G.H. Gilmer, Hanchen Huang, and Christopher Roland. Thin film deposition: fundamentals and modeling. *Computational Materials Science*, 12:354–380, 1998 **Review article on thin film deposition methods; useful when discussing high throughput investigations.**

- Christian Gobert, Edward W. Reutzel, Jan Petrich, Abdalla R. Nassar, and Shashi Phoha. Application of supervised machine learning for defect detection during metallic powder bed fusion additive manufacturing using high resolution imaging. *Additive Manufacturing*, 21:517–528, May 2018 **Study of computer vision and machine learning methods for predicting pore/inclusion formation during LPBF process; compares images taken during different layer manufacture to slices in an XCT of the finished part; classifies layers as having a defect or not using a support vector machine.**

  - **In situ**
  - **Computer vision**

- Xibing Gong and Kevin Chou. Phase-field modeling of microstructure evolution in electron beam additive manufacturing. *Journal of Materials*, 67(5):1176–1182, 2015 **Phase field model of EBAM process; specifically looking at microstructure evolution; solidification of Ti-6Al-4V; looked at effect of undercooling on dendrite growth.**

  - **Phase field microstructure evolution, solidification**
  - **ICME model**

- Abhijith M Gopakumar, Prasanna V Balachandran, Dezhen Xue, James E Gubernatis, and Turab Lookman. Multi-objective optimization for materials discovery via adaptive design. *Nature Scientifi Reports*, 8, February 2018 **Use of Maximin algorithm to predict multiple material properties from composition, specifically in the form of Pareto fronts, Ashby-chart like plots; dense in theory.**

- Michael Gouge, Pan Michaleris, Erik Denlinger, and Jeff Irwin. *Thermo-Mechanical Modeling of Additive Manfuacturing, Chapter 2: The Finite Element Method for the Thermo-Mechanical Modeling of Additive Manufacturing Processes.* Elsevier Inc, 2018 **Review of AM processes and modeling efforts behind them; specific to finite element methods.**
  - **FE Review for AM modeling**
  - **ICME**
- John J. Grefenstette. Optimization of control parameters for genetic algorithms. *IEEE Transactions of Systems, Man, and Cybernetics*, 16(1), January/February 1986 **Use of a genetic algorithm to teach a machine to perform a generic optimization task.**
- Nannan Guo and Ming C. Leu. Additive manufacturing: Technology, applications and research needs. *Frontiers of Mechanical Engineering*, 8(3):215–243, 2013 **A review of AM processes and challenges.**
- Gus L. W. Hart, Volker Blum, Michael J. Walorski, and Alex Zunger. Evolutionary approach for determining first-principles hamiltonians. *Nature Materials*, 4(5):391–394, 2005 **Uses a genetic algorithm to find model-accurate coarse grained Hamiltonians of many body systems; relevant to crystal structure prediction and material design.**
- Geoffroy Hautier, Christopher C. Fischer, Anubhav Jain, Tim Mueller, and Gerbrand Ceder. Finding natures missing ternary oxide compounds using machine learning and density functional theory. *Chemistry of Materials*, 22(12):3762–3767, 2010 **Uses the cumulant distribution function of Fischer et al. to perform a search through a database of ab initio generated crystal structures.**
  - **Alloy Design**
- B J Hayes, B W Martin, B Welk, S Kuhr, T K Ales, D A Brice, I Ghamarian, A H Baker, C V Haden, G Harlow, H L Fraser, and P C Collins. Predicting tensile properties of Ti-6Al-4V produced via directed energy deposition. *Acta Materialia*, 133:120–133, 2017 **Develops a model to predict tensile strength of wire feed AM Ti-6Al-4V from process parameters; presents constitutive equations.**
- E. Hernandez-Nava, C. J. Smith, F. Derguti, S. Tammas-Williams, F. Loonard, P. J. Withers, I. Todd, and R. Goodall. The effect of density and feature size on mechanical properties of isostructural metallic foams produced by additive manufacturing. *Acta Materialia*, 85:387–395, 2015 **Investigation of metallic foams (similar to lattice structures) produced via additive manufacturing.**
- Kai-Ming Ho, Alexandre A. Shvartsburg, Bicai Pan, Zhong-Yi Lu, Cai-Zhuang Wang, Jacob G. Wacker, James L. Fye, and Martin F. Jarrold. Structures of medium-sized silicon clusters. *Nature (London)*, 392(6676):582–585, 1998 **Uses a genetic algorithm to find the stable crystal structure for clusters of silicon.**
  - **Alloy Design**
- P. Hohenberg and W. Kohn. Inhomogenous electron gas. *Phyiscal Review*, 7(5):1912–1919, 1965 **A seminal paper on Hohenberg-Kohn-Sham DFT.**
- In Mei Li, Carelyn Campbell, Katsuyo Thornton, Elizabeth Holm, and Peter Gumbsch, editors, *Proceedings of the 2nd World Congress on Integrated Computational Materials Engineering (ICME)*, Salt Lake City, UT, July 2013. TMS (The Minerals Metals, and Materials Society) **Conferences proceedings from the World Congress on ICME.**
  - **ICME**
- Yuichi Ikeda. A new method of alloy design using a genetic algorithm and molecular dynamics simulation and its application to nickel-based superalloys. *Materials Transactions*, 38(9):771–779, 1997 **Use a genetic algorithm to design an alloy composition with specific material properties; has a great motivation/intuition for setting up GAs to achieve a desired optimization condition.**
  - **Alloy Design**

- Anubhav Jain, Geoffroy Hautier, Charles J. Moore, Shyue Ping Ong, Christopher C. Fischer, Tim Mueller, Kristin A. Persson, and Gerbrand Ceder. A high-throughput infrastructure for density functional theory calculations. *Computational Materials Science*, 50(8):2295–2310, 2011 **Outlines the infrastructure for DFT calculations and machine learning on DFT results; infrastructure would later become Materials Project; has good discussion of how certain mathematical properties in crystal structure representation are amenable to machine learning algorithms.**

- Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, and Kristin A. Persson. Commentary: The materials project: A materials genome approach to accelerating materials innovation. *APL Materials*, 1(1), 2013 **Introduces the Materials Project, outline, scope, goals, etc.**

- Anubhav Jain, Geoffroy Hautier, Shyue Ping Ong, and Kristin Persson. New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships. *Materials Research Society*, 31(8), April 2016 **Application of data mining algorithms to several different materials databases.**

- Qingbo Jia and Dondong Gu. Selective laser melting additive manfuacturing of inconel 718 superalloy parts: Densificaiton, microstructure and properties. *Journal of Alloys and Compounds*, 585:713–721, October 2014 **Studies relationship of processing parameters to microstructure and some mechanical properties; looks at processing conditions impact on microstructure and properties; observed balling at lower laser energy density; found good manufacturing parameters for near-fully-dense parts; measured microhardness and wear properties.**
  - **Parametric analysis – laser parameters (power, scan speed, thus density) → density, microstructure, microhardness, oxidation resistance**

- Yaochu Jin and Bernhard Sendhoff. Pareto-based multiobjective machine learning: An overview and case studies. *IEEE Transactions of Systems, Man, and Cybernetics - Parc C: Applications and Reviews*, 38(3), May 2008 **Theory paper on multi objective optimization; mainly discusses re-representing NN's as multiobjective optimization problems for both supervised and unsupervised tasks; relevant to fingerprint modeling section**
  - **Theory**
  - **Machine learning review**
  - **Multiobjective optimization**

- G. H. Jóhannesson, T. Bligaard, A. V. Ruban, H. L. Skriver, K. W. Jacobsen, and J. K. Norskov. Combined electronic structure and evolutionary search approach to materials design. *Physical Review Letters*, 88(25):2555061–2555065, 2002 **Uses a genetic algorithm to operate on iterations of DFT simulations; specifies GA such that specific final properties can be generated.**

- Veena N Jokhakar. A Random Forest Based Machine Learning Approach For Mild Steel Defect Diagnosis. In *Computational Intelligence and Computing Research*. IEEE, December 2016 **Applies a litany of machine learning approaches to predict when defects will occur during steel manufacturing; monitors various aspects of continuous steel manufacturing process and takes measurements; used random forests, neural networks, support vector machines, and ensemble modeling to predict defect formation.**
  - **In situ monitoring**

- Surya R. Kalidindi, David B. Brough, Shengyen Li, Ahmet Cecen, Aleksandr L. Blekh, Faical Yannick P. Congo, and Carelyn Campbell. Role of materials data science and informatics in accelerated materials innovation. *Materials Research Society Bulletin*, 41, August 2016 **Basic overview of data mining and materials informatics as it relates to the Materials Genome Initiative; identifies toolsets which may be useful in integrating aspects of materials science.**

- Sergei V. Kalinin, Bobby G. Sumpter, and Richard K. Archibald. Big–deep–smart data in imaging for guiding materials design. *Nature Materials*, 14(10):973–980, 2015 **A review/progress article on how large datasets of materials microstructures/images can be used for materials design or process design; focused specifically around discovery of new materials; identifies several different machine learning algorithms.**

– **Computer vision**


- Chandrika Kamath. Data mining and statistical inference in selective laser melting. *International Journal of Advanced Manufacturing Technology*, 10, 2016 **Uses a data-driven surrogate model to identify important variables for certain final properties in SLM; varies the laser parameters, the powder bed parameters (bed thickness, particle size, etc,), and material properties (alloy); approach is to find areas of design space which produce melt pools of appropriate geometry; performed regression using random forests to predict melt pool depths.**

- Saad A. Khairallah, Andrew T. Anderson, Alexander Rubenchik, and Wayne E. King. Laser powder bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones. *Acta Materialia*, 108:36–45, 2016 **Study on recoil pressure and Marangoni convection in LPBF of 316L SS; Looks at particle melting, partial melting, and pore formation; also investigates denudation zone near laser path; discusses remedies to these problems.**

  – **Melt pool, powder model**

  – **ICME**

- Amir Mahyar Khorasani, Ian Gibson, Umar Shafique Awan, and Alireza Ghaderi. The effect of slm process parameters on density, hardness, tensile strength and surface quality of ti-6al-4v. *Additive Manufacturing*, March 2018 **Introduces the Taguchi method of experimental design; used design of experiments to compare processing parameters (laser power, scan speed, hatch space, laser pattern angle coupling, post processing) to material properties (density, strength, elongation, average surface area).**

  – **Parametric analysis – laser parameters (above) → material properties (above)**

- C. Kim, G. Pilania, and R. Ramprasad. From organized high-throughput data to phenomenological theory using machine learning: the example of dielectric breakdown. *Chemistry of Materials*, 28(5):1304–1311, 2016 **This appears to be a paper which used random forests on a large dataset to predict dialetric breakdown.**

- Edward Kim, Kevin Huang, Alex Tomala, Sara Matthews, Emma Strubell, Adam Saunders, Andrew McCallum, and Elsa Olivetti. Data descriptor: Machine-learned and codified synthesis parameters of oxide materials. *Nature Scientific Data*, 4, September 2017 **Presents a dataset of synthesis parameters for materials; for use in conjunction with machine learning of material structures from ab initio DFT.**

- Wayne E. King, Holly D. Barth, Victor M. Castillo, Gilbert F. Gallegos, John W. Gibbs, Douglas E. Hahn, Chandrika Kamath, and Alexander M. Rubenchik. Observation of keyhole-mode laser melting in powder-bed fusion additive manufacturing. *Journals of Materials Processing Technology*, 214:2915–2925, June 2014 **Ex situ analysis of single tracks builds of LPBF; varied the energy density of the laser in different deposition; characterized the transition between conduction-mode melting and keyhole-mode melting based on incident energy density.**

- W. E. King, A. T. Anderson, R. M. Ferencz, N. E. Hodge, C. Kamath, S. A. Khairallah, and A. M. Rubenchik. Laser powder bed fusion additive manufacturing of metals; physics, computational, and materials challenges. *Applied Physics Reviews*, 2(4):041304, 2015 **This is a massive review article on the physics, modeling, and materials science of LPBF; truly a huge resource.**

  – **ICME Review for LPBF**

- W. King, A.T. Anderson, R.M. Ferencz, N.E. Hodge, C. Kamath, and S.A. Khairallah. Overview of modelling and simulation of metal powder bed fusion process at lawrence livermore national laboratory. *Materials Science and Technology*, 31(8), 2015 **Title says it all; a review of modeling of AM at LLNL.**

- Scott Kirklin, Bryce Meredig, and Chris Wolverton. High-throughput computational screening of new Li-Ion battery anode materials. *Advanced Energy Materials*, 3(2):252–262, 2013 **A high throughput combinatorial investigation of stable structures for use as anode materials; screening/search algorithm called grand canonical linear programming was used.**

- S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi. Optimization by simulated annealing. *Science*, 220:671–680, 1983 **This article describes optimization by simulated annealing for DFT.**

- W. Kohn and L.J. Sham. Self-consistent equations including exchange and correlation effects. *Physical Review*, 140, 1965 **Seminal paper on Hohenberg-Kohn-Sham DFT.**

- Hideomi Koinuma and Ichiro Takeuchi. Combinatorial solid-state chemistry of inorganic materials. *Nature Materials*, 3:429–438, 2004 **This is a review of combinatorial (high throughput ab initio) approaches to designing materials; covers both analysis methods and manufacturing methods for screening material properties; focus on inorganic functional materials.**

- Aleksey N. Kolmogorov and Stefano Curtarolo. Prediction of different crystal structure phases in metal borides: A lithium monoboride analog to Mg B2. *Physical Review B - Condensed Matter and Materials Physics*, 73(18):1–4, 2006 **Performs an ab initio screening of stable structures for a specific subset of materials – layered metal borides.**

- A.J. Kulkarni, K. Krishnamurthy, S.P. Deshmukh, and R.S. Mishra. Microstructrual optimization of alloys using a genetic algorithm. *Materials Science and Engineering A*, 372:213–220, December 2004 **A good study of how prior mat sci knowledge can be used to set up a machine learning study efficiently and in an interpretable way; uses previously developed theoretical and phenomenological models to design microstructures with specific material properties using genetic algorithms; materials by design.**

- Julia Kundin, Leslie Mushongera, and Heike Emmerich. Phase-field modeling of microstruction formation during rapid solidification in inconel 718. *Acta Materialia*, 95:343–356, 2015 **Phase field modeling of rapidly solidifying Inconel 718; evaluates a phenomenological model of dendrite growth as a function of undercooling.**
  - **Parametric analysis with a model – constitutional undercooling → dendrite arm spacing**
  - **Phase field**
  - **ICME**

- Aaron Gilad Kusne, Tieren Gao, Apurva Mehta, Liqin Ke, Manh Cuong Nguyen, Kai-Ming Ho, Vladimir Antropov, Cai-Zhuang Wang, Matthew J. Kramer, Christian Long, and Ichiro Takeuchi. On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets. *Scientific Reports*, 4(1):6367, 2015 **Not quite sure if this will actually make it into the review; they apply an algorithm called mean shift theory in order to perform on-the-fly analysis of diffraction results from a combinatorial library of synethsized materials; they were looking for a rare-earth free permanent magnet.**

- Ohyung Kwon, Hyung Giun Kim, Min Ji Ham, Wonrae Kim, Gun-Hee Kim, Jae-Hyung Cho, Nam Il Kim, and Kamgil Kim. A deep neural network for classification of melt-pool images in metal additive manfuacturing. *Journal of Intelligent Manufacturing*, October 2018 **Used a deep neural network to classify melt pool images; database of images was taken across 6 different laser power levels; the study is more concerned with training a successful NN than the AM or mat sci of the problem.**

- S.G. Lambrakos and K.P. Cooper. A general algorithm for inverse modeling of layer-by-layer liquid-metal deposition. *Journal of Materials Engineering and Performance*, 19:314–324, April 2010 **Presents a model for inverse modeling of heat transfer in layer-by-layer deposition processes; aimed toward prediction of temperature histories of final parts based on geometry.**

- Gregory A. Landrum and Hugh Genin. Application of machine-learning methods to solid-state chemistry: Ferromagnetism in transition metal alloys. *Journal of Solid State Chemistry*, 176(2):587–593, 2003 **Uses decision trees in order to predict whether or not ordered/disordered phases are ferromagnetic.**
  - **Alloy Design**

- Matthijs Langelaar. Topology optimization of 3d self-supporting structures for additive manufacturing. *Additive Manufacturing*, 12:60–70, June 2016 **A topology optimization algorithm which takes constraints of AM specifically into mind; excludes geometries which are impossible to manufacture in AM (unsupported structures); compared with traditional topology optimization algorithms.**
  - **Topology optimization**

- Matthijs Langelaar. An additive manufacturing filter for topology optimization of print-ready designs. *Structural and Multidisciplinary Optimization*, 55:871–883, July 2017 **Improvement over the algorithm presented in [Lan16] from what I can tell.**
  - **Topology optimization**
- K. F. Leong, C. M. Cheah, and C. K. Chua. Solid freeform fabrication of three-dimensional scaffolds for engineering replacement tissues and organs. *Biomaterials*, 24(13):2363–2378, 2003 **This paper prospects using solid freeform fabrication to produce biomedical devices.**
- Yali Li and Dongdong Gu. Parametric analysis of thermal behavior during selective laser melting additive manufacturing of aluminum alloy powder. *Materials and Design*, 63:856–867, 2014 **Parametric analysis of processing conditions on thermal history of SLM; finite element model; specifically looking at effects of laser power and scan speed on cooling rate and solidification velocity; also looked at wettability of melt pools and the formation of micropores; compared with prints made at same processing conditions as model.**
  - **Parametric analysis – laser parameters (above) → thermal history**
  - **FE Model**
  - **ICME**
- Julia Ling, Max Hutchinson, Erin Antono, Sean Paradiso, and Bryce Meredig. High-Dimensional Materials and Process Optimization using Data-driven Experimental Design with Well-Calibrated Uncertainty Estimates. *Integrating Matereials and Manufacturing Innovation*, 6:207–217, 2017 **Outlines the backbone of Citrines recommendation system for experiments; uses sequential learning approach based on random forests; found the optimal choice with three times fewer tests needed.**
- Julia Ling, Maxwell Hutchinson, Erin Antono, Brian DeCost, Elizabeth A. Holm, and Bryce Meredig. Building data-driven models with microstructural images: Generalization and interpretability. *Materials Discovery*, 10:19–28, 2017 **This paper details the use of convolutional neural networks for classify microstructures; generalized some aspects of classifying microstructure images.**
- Zi-Kui Liu, Long-Qing Chen, and Krishna Rajan. Linking length scales via materials informatics. *Journal of Materials: Integrated Computational Materials*, pages 42–51, November 2006 **Pretty early paper on machine learning of database information, specifically DFT and CALPHAD based modeling; informatics approach used is linear regression.**
- Rouqian Liu, Abhishek Kumar, Zhengzhang Chen, Ankit Agrawal, Veera Sundaraghavan, and Alok Choudhary. A predictive machine learning approach for microstructure optimization and materials design. *Nature Scientific Reports*, 5, June 2015 **This is a machine learning approach to inverse design of microstructures, optimizing on magnetic properties; framework involves random data generation, feature selection, and classification; algorithms used include maximum likelihood, genetic algorithm, exhaustive search, better than random guided search, and linear programming.** A good paper to read through thoroughly.
- C. J. Long, J. Hattrick-Simpers, M. Murakami, R. C. Srivastava, I. Takeuchi, V. L. Karen, and X. Li. Rapid structural mapping of ternary metallic alloy systems using the combinatorial approach and cluster analysis. *Review of Scientific Instruments*, 78(7), 2007 **They use PCA on a dataset of microdiffraction results to find characteristic XRD patterns for a given material system; they then rapidly identify new material systems based on a PCA analysis of their microdiffraction patterns.**
  - **Matrix factorization**
  - **Dimensionality reduction**
- C. J. Long, D. Bunker, X. Li, V. L. Karen, and I. Takeuchi. Rapid identification of structural phases in combinatorial thin-film libraries using x-ray diffraction and non-negative matrix factorization. *Review of Scientific Instruments*, 80(10), 2009 **Uses non-negative matrix factorization to rapidly classify a dataset of microdiffraction patterns; compared with PCA results from [LHSM+07]; provides a more interpretable dimensionality reduction of microdiffraction patterns.**
  - **Matrix factorization**

  - **Dimensionality reduction**

- David G. Lowe. Distinctive image features from scale-invariant keypoints. *International Journal of Computer Vision*, 60(2):91–110, November 2004 **An original paper on SIFT.**

  - **Computer vision**

- Xufei Lu, Xin Lin, Michele Miumenti, Miguel Cervera, Yunlong Hu, Xianglin Ji, Liang Ma, and Weidong Huang. In-situ measurements and thermo-mechanical simulation of ti-6al-4v laser solid forming processes. *International Journal of Mechanical Sciences*, January 2019 **A thermomechanical models of the laser cladding process of Ti-6Al-4V;**

  - **Process modeling**
  - **Laser cladding Ti-6Al-4V**

- Nicholas Lubbers, Turab Lookman, and Kipton Barros. Inferring low-dimensional microstructure representations using convolutional neural networks. pages 1–25, 2016 **Study on using pre-trained convolutional neural networks to characterize synthetic microstructure images; uses manifold learning to embed characterizations into low-dimensional space; low-dimensional embedding reveals information about parameters which generated the images; could be applied to real microstructures maybe?**

  - **Computer vision**

- Mahesh Mani, Brandon M. Lane, M. Alkan Donmez, Shaw C. Feng, and Shawn P. Moylan. A review on measurement science needs for real-time control of additive manufacturing metal powder bed fusion processes. *International Journal of Production Research*, 55(5), August 2017 **A review on needs for in situ feedback and control; focused on feed-forward and closed-loop monitoring of AM systems.**

  - **In situ monitoring**

- Arun Mannodi-Kanakkithodi, Ghanshyam Pilania, Tran Doan Huan, Turab Lookman, and Rampi Ramprasad. Machine learning strategy for accelerated design of polymer dialetricsc. *Nature Scientific Reports*, 6:1–10, February 2016 **Uses fingerprint methods (including a genetic algorithm) for design of polymer chains to be used as dialetric material; Nature Scientific Reports article**

  - **Alloy design**
  - **Materials design**

- V. Manvatkar, A. De, and T. DebRoy. Heat transfer and material flow during laser assisted multi-layer additive manufacturing. *Journal of Applied Physics*, 116, September 2014 **Investigation of spatial variation of melt pool geometry, cooling rate, peak temperature in various layers throughout a LENS build; used cooling rates and solidification parameters to predict hardness; compared with experimental results.**

- John H. Martin, Brennan D. Yahata, Jacob M. Hundley, Justin A. Mayer, Tobias A. Schaedler, and Tresa M. Pollock. 3d printing of high-strength aluminum alloys. *Nature Letters*, 549:365–370, September 2017 **This paper details the design of an aluminum alloy specifically for additive manufacturing; they used a random search to find lattice-matched nucleants for aluminum alloys.**

  - **Alloy Design**

- Richard Martukanitz, Pan Michaleris, Todd Palmer, Tarasankar DebRoy, Zi-Kiu Liu, Richard Otis, Tae Wook Heo, and Long-Qing Chen. Toward an integrated computational system for describing the additive manufacturing process for metallic materials. *Addtive Manufacturing*, 1(4):52–63, August 2014 **Presents an ICME approach to modeling AM; model incorporates thermal, mechanical, and material responses during manufacturing; discusses process maps, impacts of energy density on solidification, heat transfer in models, mass transfer in models, solid state phase transformations which occur during manufacturing.**

  - **Full ICME approach**

- Joseph T. McKeown, Kai Zweiacker, Can Liu, Daniel R Coughlin, Amy J Clarke, J Kevin Baldwin, John W Gibbs, John D Roehling, SEth D Imhoff, Paul J Gibbs, Damien Tourret, Jörg M.K. Wiezorek, and Geoffrey H Campbell. Time-resolved in situ measurements during rapid alloy solidification: Experimental insight for additive manufacturing. *JOM*, 68(3), 2016 **In situ investigation of solidification velocities for rapidly solidifying Al-Cu alloys; performed dynamic TEM to observe solidification front, microstructure evolution, and instability at liquid-solid interface.**
  - **In situ monitoring**
- Pankaj Mehta, Ching-Hao Wang, Alexandre G.R. Day, Clint Richardson, Marin Bukov, Charles K. Fisher, and David J. Schwab. A high-bias, low-variance introduction to machine learning for physicists. *arxiv PrePrint*, 2018 **An arXiv preprint with reviews of many, many different machine learning algorithms.**
- Stephen Mellor, Liang Hao, and David Zhang. Additive manufacturing: A framework for implementation. *International Journal of Production Economics*, 149:194–201, 2014 **Perspective for implementing AM at a wide scale from a socio-technical perspective; identifies personnel infrastructure which needs to be in place for AM to succeed.**
- B. Meredig, A. Agrawal, S. Kirklin, J. E. Saal, J. W. Doak, A. Thompson, K. Zhang, A. Choudhary, and C. Wolverton. Combinatorial screening for new materials in unconstrained composition space with machine learning. *Physical Review B - Condensed Matter and Materials Physics*, 89(9):1–7, 2014 **Application of ensembles of decision trees to predict formation energies of various materials; compares the results with DFT simulations.**
- National science and technology council, office of science and technology policy, materials genome initiative for global competitiveness, 2011 **A white paper on the materials genome initiative.**
- Panagiotis Michaleris. Modeling metal deposition in heat transfer analyses of additive manufacturing processes. *Finite Elements in Analysis and Design*, 86:51–60, April 2014 **Finite element model developed for studying heat transfer in a generalized layer-by-layer AM system; uses inactive and active elements for model; looks at heat transfer as wall is built up.**
  - **FE thermomechanical model**
  - **ICME**
- Nele Moelans, Bart Blanpain, and Patrick Wollants. An introduction to phase-field modeling of microstructure evolution. *Computer Coupling of Phase Diagrams and Thermochemistry*, 32:268–294, 2008 **A review on phase field modeling approaches to microstructure evolution.**
- Dane Morgan, Gerbrand Ceder, and Stefano Curtarolo. High-throughput and data mining with <i>ab initio</i> methods. *Measurement Science and Technology*, 16(1):296–301, 2005 **Discusses some of the challenges with setting up high through ab initio investigations in DFT. Discusses data mining techniques to find formation energies and stable crystal structures.**
- J. Morris, D. Deaven, and K. Ho. Genetic-algorithm energy minimization for point charges on a sphere. *Physical Review B*, 53(4):R1740–R1743, 1996 **Cleverly applies a genetic algorithm approach to the problem of finding the minimum energy stable configuration of N many electronic charges; extends up to** $N = 200$**; good paper for demonstrating how carefully considering you problem in relation to the algorithm architecture can aid in success of applying machine learning.**
- National institute of materials science, July 2017 **Citation for Japan's National Institute of Materials Science.**
- Pulin Nie, O.A. Ojo, and Zhuguo Li. Numerical modeling of microstructure evolution during laser additive manufacturing of a nickel-based superalloy. *Acta Materialia*, 77:85–95, 2014 **Finite element and stochastic analysis models used to study microstructure evolution of a nickel-based superalloy (Nb stabilized, so its probably 615 or 718); studies nucleation and growth of dendrites, Nb segregation, laves phase formation; evaluated relationship between temperature gradient (G) and solidification velocity (R) and the dendrite arm spacing, distribution of laves phase, tendency to hot crack.**
  - **Parametric analysis – temperature history (gradient, rates)** $\rightarrow$ **dendrite arm spacing**
  - **FE model**

  - **ICME**

- Artem R. Oganov and Colin W. Glass. Crystal structure prediction using ab initio evolutionary techniques: Principles and applications. *Journal of Chemical Physics*, 124(24), 2006 **An early application of genetic algorithms/evolutionary algorithms on ab initio DFT searches; starts with a database of ab initio total energy calculations, uses evolutionary algorithm to find stable crystal structure.**

  - **Alloy Design**

- Roberto Olivares-Amaya, Carlos Amador-Bedolla, Johannes Hachmann, Sule Atahan-Evrenk, Roel S. Sánchez-Carrera, Leslie Vogt, and Alán Aspuru-Guzik. Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. *Energy & Environmental Science*, 4(12):4849, 2011 **Application of multiple linear regression on a database of material properties for prediction of photovoltaic materials.**

- A.O. Oliynyk, E. Antono, T.D. Sparks, L. Ghadbeigi, M.W. Gaultois, B. Meredig, and A. Mar. High-throughput machine-learning-driven synthesis of full-Heusler compounds. *Chemistry of Materials*, 28(20):7324–7331, 2016 **Paper that uses ensemble modeling for prediction of Heusler compounds.**

  - **Alloy design**

- Runhai Ouyang, Stefano Curtarolo, Emre Ahmetcik, Matthias Scheffler, and Luca M. Ghiringhelli. Sisso: a compressed sensing method for systematically identifying efficient physical models of materials properties. *arXiv PrePrint* **This paper presents sure independence screening and sparsifying operators (SISSO) which is a method of descriptor analysis; algorithm takes a set of starting descriptors and mathematical operations and creates new descriptors out of combinations of the original set; uniqueness of the approach is that it limits the descriptors which can be formed based on dimensional analysis i.e. the physical dimension of the new descriptor must make sense.**

- Deepankar Pal, Nachiket Patil, Kai Zeng, and Brent Stucker. An integrated approach to additive manufacturing simulations using physics based, coupled multiscale process modeling. *Journal of Manufacturing Science and Engineering*, 136:1–16, December 2014 **They present a thermomechanical finite element model that is faster and more robust (they claim) than other approaches; their target is toward verifying in situ close loop process control and for predicting residual stress or distortion build up.**

  - **FE thermomechanical model**
  - **ICME**

- Ghanshyam Pilania, Chenchen Wang, Xun Jiang, Sanguthevar Rajasekaran, and Ramamurthy Ramprasad. Accelerating materials property predictions using machine learning. *Scientific Reports*, 3(1):2810, 2013 **Paper is focused on material property prediction based on stable crystal structure; uses fingerprint representation of chemo-structural characteristics and electronic charge density to screen for materials; discovers 'selection rules' for given material properties based on characteristics of fingerprints.**

- A. Plotkowski, M.M. Kirka, and S.S. Babu. Verificaiton and validation of a rapid heat transfer calculation methodology for transient melt pool solidification conditions in powder bed metal additive manufacturing. *Additive Manufacturing*, 18:256–268, 2017 **Proposes an approach to predict transient heat conduction during e-beam PBF; looks at melt pool geometry and solid-liquid interface velocity; experimentally validated on IN718.**

- Tomaso Poggio, Ryan Rifkin, Sayan Mukherjee, and Partha Niyogi. General conditions for predictivity in learning theory. *Nature*, 428(6981):419–422, 2004 **Very technical paper on the necessary conditions for certain classes of learners to be successful.**

- David Poole. *Linear Algebra: A Modern Introduction*, volume 1. Brookes/Cole, Cengage Learning, 20 Channel Center Street, Boston, MA 02210 USA, 2011 **Nate's favorite book from undergrad.**

- J.R. Quinlan. Induction of decision trees. *Machine Learning*, 1:81–106, 1986 **A text on decision trees.**

- Narendran Raghavan, Ryan Dehoff, Sreekanth Pannala, Srdjan Simunovic, Michael Kirka, John Turner, Neil Carlson, and Sudarsanam S. Babu. Numerical modeling of heat-transfer and the influence of process parameters on tailoring the grain morphology of in718 in electron beam additive manufacturing. *Acta Materialia*, 112:303–314, April 2016 **Looking at transient thermal behavior as AM parts are heated and re-heated during layerwise manufacturing; looked at spatial and temporal evolution of temperature gradient (G) and solidification velocity (R); characterized thermal history based on electron beam parameters; analyzed conditions necessary for a columnar-to-equiaxed transition; validated using experimental results.**
  - **FE thermomechanical model**
  - **ICME**
- Rampi Ramprasad, Rohit Batra, Ghanshyam Pilania, Arun Mannodi-Kanakkithodi, and Chiho Kim. Machine learning in materials informatics: recent applications and prospects. *Nature Computational Materials*, 3(54), 2017 **Review article on machine learning in materials science; covers successful studies undertaken in the past decade; looks specifically at fingerprints or descriptors of material systems; describes learning approaches based on types of material descriptors and the level of the descriptor (material level, molecular level, atomic level).**
- J. Raplee, A. Plotkowski, M. M. Kirka, R. Dinwiddie, A. Okello, R. R. Dehoff, and S. S. Babu. Thermographic microstructure monitoring in electron beam additive manufacturing. *Scientific Reports*, 7:1–16, March 2017 **Focused around process monitoring of electron beam powder bed fusion; calibrates temperature profiles from thermographic data; observes temperatures during transition between solid and liquid during manufacture.**
  - **In situ monitoring**
- Sam T. Roweis and Lawrence K. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290, December 2000 **A primer on a non linear dimensionality reduction technique.**
  - **Dimensionality reduction**
- Anindya Roy, Joseph W. Bennett, Karin M. Rabe, and David Vanderbilt. Half-heusler semiconductors as piezoelectrics. *Physical Review Letters*, 109(3):1–5, 2012 **A paper on ab initio methods for finding half heusler compounds.**
  - **Alloy design**
- Arman Sabbaghi and Qiang Huang. Predictive model building across different process conditions and shapes in 3D printing. *IEEE International Conference on Automation Science and Engineering*, 2016-Novem:774–779, 2016 **Develops a Bayesian inference approach for predicting deformation that occurs during 3D printing.**
- Seshadev Sahoo and Kevin Chou. Phase-field simulation of microstructure evolution of ti-6al-4v in electron beam additive manufacturing process. *Additive Manufacturing*, 9:14–24, December 2016 **Phase field study of Ti-6Al-4V microstructure growth in electron beam powder AM. Looks at growth of dendrite arms as a function of temperature gradient; ignores crystallographic information, does not distinguish between nucleating phases during solidification; reports temperature gradients, which could be useful for in situ Ti-6Al-4V diffraction study; outlines some equations behind phase field modeling pretty well.**
  - **Phase field dendrite growth**
  - **ICME**
- W.J. Sames, F.A. List, S. Pannala, R.R. Dehoff, and S.S. Babu. The metallurgy and processing science of metal additive manufacturing. *International Materials Reviews*, 61(5):315–362, March 2016 **Review of techniques for processing and metallurgy of AM; covers processing defects, heat transfer, solidification, solid-state precipitation, mechanical properties and post-processing metallurgy.A good review to read.**

- K. T. Schütt, H. Glawe, F. Brockherde, A. Sanna, K. R. Müller, and E. K U Gross. How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. *Physical Review B - Condensed Matter and Materials Physics*, 89(20):1–5, 2014 This is a great article that should be highlighted up front in the final draft. **This article applies KRR to predicting the density of electronic states above the Fermi energy using a novel crystal structure representation; they use radial basis functions defined in terms of the neighborhood distance of different atoms in the unit cell; they define it for a unit cell with two atoms, could easily be extended to $\mathbb{R}^3$ and higher; high prediction accuracy.**

- Luke Scime and Jack Beuth. A multi-scale convolutional neural network for autonomous anomaly detection and classification in a laser powder bed fusion additive manufacturing process. *Additive Manufacturing*, 24:273–286, October 2018 **Study using a CNN to autonomously detect and classify anomalies in a LPBF process; it looks like it was fairly effective; optical light camera mounted overhead of powder bed took images during printing; CNN was able to identify anomalies such as recoater hopping, recoater streaking, debric, super-elevation, part damage, and incomplete spreading at accuracies over 70% for all using a Multi-scale CNN (MsCNN).**
  - **In situ monitoring**
  - **Computer vision**

- J M Serra, L A Baumes, M Moliner, P Serna, and A Corma. Zeolite synthesis modelling with support vector machines: A combinatorial approach. *Combinatorial Chemistry & High Throughput Screening*, 10(1):13–24, 2007 **Applies support vector machines (SVM) to predict zeolite synthesis based on starting gel compositions and weight ratios; compared SVM to NN and classification trees.**
  - **Alloy design**

- Wahyu Setyawan and Stefano Curtarolo. High-throughput electronic band structure calculations: Challenges and tools. *Computational Materials Science*, 49(2):299–312, 2010 **This presents a study on bottlenecks in high throughput band structure calculation from DFT; looks like its a case study in using AFLOW.**

- Wahyu Setyawan, Romain M Gaume, Stephanie Lam, Robert S Feigelson, and Stefano Curtarolo. High-Throughput Combinatorial Database of Electronic Band Structures for Inorganic Scintillator Materials. *ACS Combinatorial Science*, pages 382–390, 2011 **Demonstration of AFLOW on predicting the band structure of 7439 materials to search for a good scintillator for $\gamma$ ray radiation detection.**

- Songqing Shan and G. Gary Wang. Survery of modeling and optimization strategies to solve high-dimensional design problems iwth computationall-expsive black-box functions. *Structural and Multidisciplinary Optimization*, 41:219–241, November 2010 **This is a survey of papers focused on: strategies for tackling the high dimensionality of problems, model approximation techniques, and direct optimization strategies for computationally-expensive black-box functions and promising ideas behind non-gradient optimization algorithms.** Could be a good resource to point people toward when discussing more theoretical considerations.

- Claude E Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27(July 1928):379–423, 1948 **Seminal paper in information theory.**

- John C. Snyder, Matthias Rupp, Katja Hansen, Klaus Robert Müller, and Kieron Burke. Finding density functionals with machine learning. *Physical Review Letters*, 108(25):1–5, 2012 **Application of machine learning to predict electron density functions a la Kohn-Sham DFT; uses PCA on a dataset of functionals to predict other functionals.**

- Giovanni Strano, Liang Hao, Richard M. Everson, and Kenneth E. Evans. Surface roughness analysis, modelling, and prediction in selective laser melting. *Journal of Material Processing Technology*, 21:589–597, 2013 **Surface roughness analysis, modeling, and prediction for 316L SS produced via SLM; develops a model for predicting surface roughness which takes into account unmelted particles on the surface; model is based on geometric setup of the build.**
  - **Parametric analysis – geometry/orientation $\rightarrow$ surface roughness**

- David P. Stucke and Vincent H. Crespi. Predictions of new crystalline states for assemblies of nanoparticles: Perovskite analogues and 3-D arrays of self-assembled nanowires. *Nano Letters*, 3(9):1183–1186, 2003 **Applies a genetic search algorithm to optimize packing density of crystal nanoparticles.**

- B G Sumpter and D W Noid. On the Design, Analysis, and Characterization of Materials Using Computational Neural Networks. *Annual Review of Materials Science*, 26(1):223–277, 1996 **A review of convolutional neural networks and their applications in materials science through 1996. Probably the earliest work on machine learning in materials science I've found yet.**

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