Atomic Parameters

Quantities will be normalized vs hydrogen

```
hydrogenAtomicRadius = N[QuantityMagnitude[ElementData[1, "AtomicRadius"]]] 53.  
hydrogenAtomicCrossSection = \pi * hydrogenAtomicRadius² 8824.73  
hydrogenAtomicVolume = \frac{4\pi}{3} * hydrogenAtomicRadius³ 623 615.
```

Grabbing all other quantities

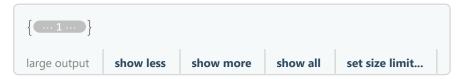
```
atomicRadii =
    {#, N[QuantityMagnitude[ElementData[#, "AtomicRadius"]]]} & /@ {26, 14, 6, 13, 5, 15, 31, 32,
           29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92} (* In picometers *)
 \{\{26, 156.\}, \{14, 111.\}, \{6, 67.\}, \{13, 118.\}, \{5, 87.\}, \{15, 98.\}, \{31, 136.\},
    \{32, 125.\}, \{29, 145.\}, \{47, 165.\}, \{79, 174.\}, \{30, 142.\}, \{22, 176.\},
    {23, 171.}, {24, 166.}, {40, 206.}, {41, 198.}, {42, 190.}, {72, 208.},
    {73, 200.}, {74, 193.}, {58, QuantityMagnitude[Missing[NotAvailable]]},
    {59, 247.}, {64, 233.}, {92, QuantityMagnitude[Missing[NotAvailable]]}}
atomicRadii[[22, 2]] = 248.
248.
atomicRadii[[25, 2]] = 230.
230.
atomicCrossSection =
    \left\{\#[1], \frac{\pi * \#[2]^2}{\text{hydrogenAtomicCrossSection}}\right\} \& \ / @ \ \text{atomicRadii} \ (* \ \text{In picometers squared *})
 \{\{26, 8.66358\}, \{14, 4.38626\}, \{6, 1.59808\}, \{13, 4.95692\}, \{5, 2.69455\}, \{6, 1.59808\}, \{13, 4.95692\}, \{13, 2.69455\}, \{13, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2.69455\}, \{14, 2
    \{15, 3.41901\}, \{31, 6.58455\}, \{32, 5.56248\}, \{29, 7.48487\}, \{47, 9.69206\},
     {79, 10.7782}, {30, 7.17836}, {22, 11.0274}, {23, 10.4098}, {24, 9.8099},
    {40, 15.1072}, {41, 13.9566}, {42, 12.8515}, {72, 15.4019}, {73, 14.2399},
    \{74, 13.2606\}, \{58, 21.8953\}, \{59, 21.7191\}, \{64, 19.3268\}, \{92, 18.8323\}\}
```

```
atomicVolumes = \left\{\#[1], \frac{\frac{4\pi}{3} * \#[2]^3}{\text{hydrogenAtomicVolume}}\right\} \& /@ atomicRadii (* In picometers cubed *)
 \{\{26, 25.5004\}, \{14, 9.18631\}, \{6, 2.02021\}, \{13, 11.0362\}, \{5, 4.42313\}, \{6, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2.02021\}, \{13, 2
      \{15, 6.32194\}, \{31, 16.8962\}, \{32, 13.1191\}, \{29, 20.4775\}, \{47, 30.1734\},
      \{79, 35.3851\}, \{30, 19.2326\}, \{22, 36.6193\}, \{23, 33.5862\}, \{24, 30.7253\},
      {40, 58.7184}, {41, 52.1396}, {42, 46.0716}, {72, 60.4453}, {73, 53.7356},
      {74, 48.2886}, {58, 102.454}, {59, 101.219}, {64, 84.965}, {92, 81.7252}}
atomicMasses = {#, QuantityMagnitude[ElementData[#, "AtomicMass"]]} & /@ {26, 14, 6, 13, 5,
               15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92} (* In amu *)
 \{\{26, 55.845\}, \{14, 28.085\}, \{6, 12.011\}, \{13, 26.9815385\}, \{5, 10.81\}, \{13, 26.9815385\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.085\}, \{14, 28.
      {15, 30.973761998}, {31, 69.723}, {32, 72.630}, {29, 63.546}, {47, 107.8682},
     \{79, 196.966569\}, \{30, 65.38\}, \{22, 47.867\}, \{23, 50.9415\}, \{24, 51.9961\},
     \{40, 91.224\}, \{41, 92.90637\}, \{42, 95.95\}, \{72, 178.49\}, \{73, 180.94788\},
     {74, 183.84}, {58, 140.116}, {59, 140.90766}, {64, 157.25}, {92, 238.02891}}
atomicValenceElectrons =
      {#, Total[Take[Flatten[ElementData[#, "ElectronConfiguration"]], -2]]} & /@ {26, 14, 6,
               13, 5, 15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92}
               (* Doesn't work for Cu, Ag, Au, Zn, but is okay with early transitions *)
 \{\{26, 8\}, \{14, 4\}, \{6, 4\}, \{13, 3\}, \{5, 3\}, \{15, 5\}, \{31, 3\}, \{32, 4\},
      \{29, 11\}, \{47, 11\}, \{79, 11\}, \{30, 12\}, \{22, 4\}, \{23, 5\}, \{24, 6\}, \{40, 4\},
      \{41, 5\}, \{42, 6\}, \{72, 4\}, \{73, 5\}, \{74, 6\}, \{58, 3\}, \{59, 8\}, \{64, 3\}, \{92, 3\}\}
```

Data Processing

Import Database

rawData = Import["C:\\Users\\laris\\Documents\\MIT\\2018\\Summer\\Texas Research\\Final Data\\Database Curation\\CuratedDatabase7-26.csv"]



rawLabels = rawData[1, 1;; 33]

{Fe, Si, C, Al, B, P, Ga, Ge, Cu, Ag, Au, Zn, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W, Ce, Pr, Gd, U, Annealing temperature (K), Annealing Time (s), Primary Crystallization Onset (K), Primary Crystallization Peak (K), Secondary Crystallization Peak (K), Longitudinal Annealing field, Transverse Annealing field, Ribbon Thickness (um) }

Splitting Database into Columns

```
featureColumns = rawData[2;; -1, #] & /@ Range[1, Length[rawData[1]]]]
```

```
{...1...}
large output
                show less
                               show more
                                              show all
                                                           set size limit...
```

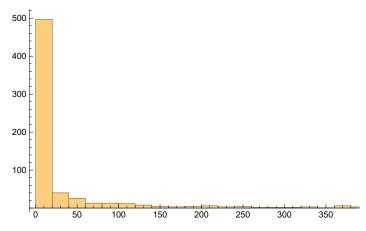
Raw Features

```
percentFe = featureColumns[1];
percentSi = featureColumns[2];
percentC = featureColumns[3];
percentAl = featureColumns[4];
percentB = featureColumns[5];
percentP = featureColumns[6];
percentGa = featureColumns[7];
percentGe = featureColumns[[8]];
percentCu = featureColumns[9];
percentAg = featureColumns[10];
percentAu = featureColumns[[11]];
percentZn = featureColumns[12];
percentTi = featureColumns[13];
percentV = featureColumns[14];
percentCr = featureColumns[15];
percentZr = featureColumns[16];
percentNb = featureColumns[17];
percentMo = featureColumns[18];
percentHf = featureColumns[19];
percentTa = featureColumns[20];
percentW = featureColumns[21];
percentCe = featureColumns[22];
percentPr = featureColumns[23];
percentGd = featureColumns[24];
percentU = featureColumns[25];
annealingTemp = featureColumns[26];
annealingTime = featureColumns[27];
primaryCrystalOnset = featureColumns[28];
primaryCrystalPeak = featureColumns[29];
secondaryCrystalPeak = featureColumns[30];
laField = featureColumns[31];
taField = featureColumns[[32]];
ribbonThickness = featureColumns[33];
rawFeatures = featureColumns[1;; 33];
earlyFeatures = {percentTi, percentV, percentCr, percentZr, percentNb, percentMo,
   percentHf, percentTa, percentW, percentCe, percentPr, percentGd, percentU};
lateFeatures = {percentCu, percentAg, percentAu, percentZn};
```

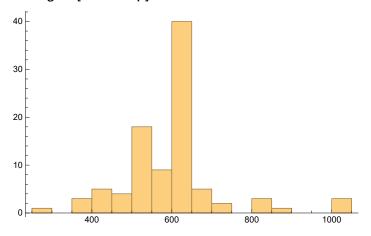
Values

```
coercivity = featureColumns[34];
curieTemp = featureColumns[35];
coreLoss = featureColumns[36];
electricalResistivity = featureColumns[37];
permeability = featureColumns[38];
magnetostriction = featureColumns[39];
magneticSaturation = featureColumns[40];
grainDiameter = featureColumns [41];
doi = featureColumns[42];
```

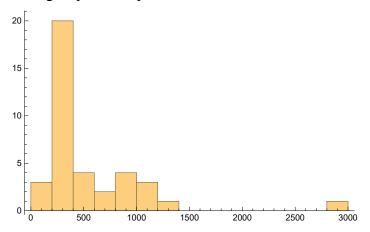
Histogram[coercivity]



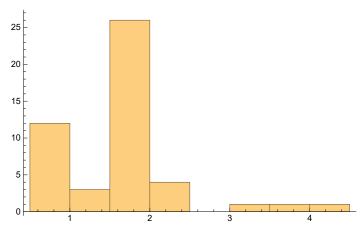
Histogram[curieTemp]



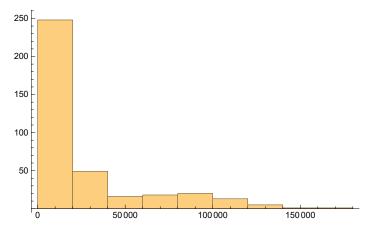
Histogram[coreLoss]



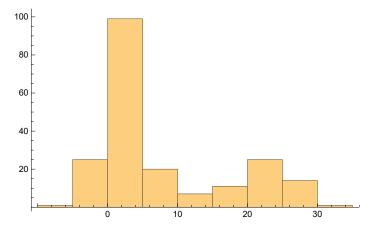
Histogram[electricalResistivity]



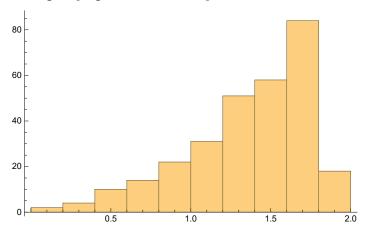
Histogram[permeability]



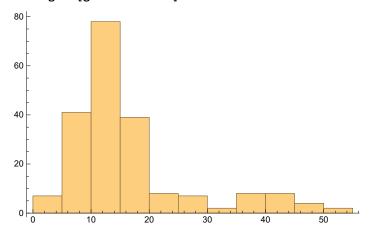
Histogram[magnetostriction]



Histogram[magneticSaturation]



Histogram[grainDiameter]



Simple Sum Transforms

```
percentSiCAl = Total[{percentSi, percentAl, percentC}, {1}];
(* Percent Si and Al and C combined *)
percentBP = Total[{percentB, percentP}, {1}];(* Percent B and P combined *)
percentGaGe = Total[{percentGa, percentGe}, {1}];(* Percent Ga and Ge combined *)
lateTransitionTotal = Total[lateFeatures, {1}];
earlyTransitionTotal = Total[earlyFeatures, {1}];
```

Simple Multiplication/Division Transforms

```
relativeToFeSiCAl = N[percentSiCAl[#]] / percentFe[#]] & /@ Range[1, Length[percentFe]];
relativeToFeBP = N[percentBP[#] / percentFe[#]] & /@ Range[1, Length[percentFe]];
relativeToFeGaGe = N[percentGaGe[#]] / percentFe[[#]] & /@ Range[1, Length[percentFe]];
relativeToFeEarlyTransition =
  N[earlyTransitionTotal[#]] / percentFe[#]] & /@ Range[1, Length[percentFe]];
relativeToFeLateTransition = N[lateTransitionTotal[#]]/percentFe[[#]] & /@
   Range[1, Length[percentFe]];
relativeToLateEarly = Quiet [N[earlyTransitionTotal[#]] / lateTransitionTotal[#]] & /@
     Range[1, Length[lateTransitionTotal]]] /. {Indeterminate → "", ComplexInfinity → ""};
relativeToEarlySiCAl = Quiet [N[percentSiCAl[#]] / earlyTransitionTotal[#]] & /@ Range [1,
       Length[earlyTransitionTotal]] /. {Indeterminate → "", ComplexInfinity → ""};
relativeToLateSiCAl = Quiet[N[percentSiCAl[#]] / lateTransitionTotal[#]] & /@
     Range[1, Length[lateTransitionTotal]] /. {Indeterminate → "", ComplexInfinity → ""};
relativeToEarlyBP = Quiet[N[percentBP[#]] / earlyTransitionTotal[#]] & /@ Range[1,
      Length[earlyTransitionTotal]]] /. {Indeterminate → "", ComplexInfinity → ""};
relativeToLateBP = Quiet[N[percentBP[#]] / lateTransitionTotal[#]] & /@
     Range[1, Length[lateTransitionTotal]]] /. {Indeterminate → "", ComplexInfinity → ""};
relativeToEarlyGaGe = Quiet[N[percentGaGe[#]] / earlyTransitionTotal[#]] & /@ Range[1,
      Length[earlyTransitionTotal]] / . {Indeterminate → "", ComplexInfinity → ""};
relativeToLateGaGe = Quiet[N[percentGaGe[#]] / lateTransitionTotal[#]] & /@
     Range[1, Length[lateTransitionTotal]] /. {Indeterminate → "", ComplexInfinity → ""};
```

Weighted Average Transforms

Volume List

```
{volume[fe],
 volume[si],
 volume[c],
 volume[al],
 volume[b],
 volume[p],
 volume[ga],
 volume[ge],
 volume[cu],
 volume[ag],
 volume[au],
 volume[zn],
 volume[ti],
 volume[v],
 volume[cr],
 volume[zr],
 volume[nb],
 volume[mo],
 volume[hf],
 volume[ta],
 volume[w],
 volume[ce],
 volume[pr],
 volume[gd],
 volume[u] = atomicVolumes[Flatten[Position[atomicVolumes, {#, _}]]][[1, 2] & /@ {26,
   14, 6, 13, 5, 15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92}
{25.5004, 9.18631, 2.02021, 11.0362, 4.42313, 6.32194, 16.8962, 13.1191,
20.4775, 30.1734, 35.3851, 19.2326, 36.6193, 33.5862, 30.7253, 58.7184,
52.1396, 46.0716, 60.4453, 53.7356, 48.2886, 102.454, 101.219, 84.965, 81.7252}
```

Cross Section List

```
{xArea[fe],
 xArea[si],
 xArea[c],
 xArea[al],
 xArea[b],
 xArea[p],
 xArea[ga],
 xArea[ge],
 xArea[cu],
 xArea[ag],
 xArea[au],
 xArea[zn],
 xArea[ti],
 xArea[v],
 xArea[cr],
 xArea[zr],
 xArea[nb],
 xArea[mo],
 xArea[hf],
 xArea[ta],
 xArea[w],
 xArea[ce],
 xArea[pr],
 xArea[gd],
 xArea[u] =
atomicCrossSection[Flatten[Position[atomicCrossSection, {#, _}]]][1, 2] & /@ {26, 14, 6,
   13, 5, 15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92}
{8.66358, 4.38626, 1.59808, 4.95692, 2.69455, 3.41901, 6.58455, 5.56248,
7.48487, 9.69206, 10.7782, 7.17836, 11.0274, 10.4098, 9.8099, 15.1072, 13.9566,
12.8515, 15.4019, 14.2399, 13.2606, 21.8953, 21.7191, 19.3268, 18.8323}
```

Mass List

```
{mass[fe],
  mass[si],
  mass[c],
  mass[al],
  mass[b],
  mass[p],
  mass[ga],
  mass[ge],
  mass[cu],
  mass[ag],
  mass[au],
  mass[zn],
  mass[ti],
  mass[v],
  mass[cr],
  mass[zr],
  mass[nb],
  mass[mo],
  mass[hf],
  mass[ta],
  {\sf mass}\,[{\sf w}] ,
  mass[ce],
  mass[pr],
  mass[gd],
  mass[u]\} = atomicMasses[Flatten[Position[atomicMasses, {\#, _}]]][1, 2] & @ {26, 14, 6, 6}
   13, 5, 15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92}
{55.845, 28.085, 12.011, 26.9815385, 10.81, 30.973761998, 69.723, 72.630,
63.546, 107.8682, 196.966569, 65.38, 47.867, 50.9415, 51.9961, 91.224, 92.90637,
95.95, 178.49, 180.94788, 183.84, 140.116, 140.90766, 157.25, 238.02891}
```

Valence Electron List

```
{vElectrons[fe],
  vElectrons[si],
  vElectrons[c],
  vElectrons[al],
  vElectrons[b],
  vElectrons[p],
  vElectrons[ga],
  vElectrons[ge],
  vElectrons[cu],
  vElectrons[ag],
  vElectrons[au],
  vElectrons[zn],
  vElectrons[ti],
  vElectrons[v],
  vElectrons[cr],
  vElectrons[zr],
  vElectrons[nb],
  vElectrons[mo],
  vElectrons[hf],
  vElectrons[ta],
  vElectrons[w],
  vElectrons[ce],
  vElectrons[pr],
  vElectrons[gd],
  vElectrons[u] =
 atomicValenceElectrons[Flatten[Position[atomicValenceElectrons, {#, _}]]][1, 2] & /@ {26,
   14, 6, 13, 5, 15, 31, 32, 29, 47, 79, 30, 22, 23, 24, 40, 41, 42, 72, 73, 74, 58, 59, 64, 92}
{8, 4, 4, 3, 3, 5, 3, 4, 11, 11, 11, 12, 4, 5, 6, 4, 5, 6, 4, 5, 6, 3, 8, 3, 3}
Late Transition Transforms
{vElectrons[cu], vElectrons[ag], vElectrons[au], vElectrons[zn]} = {2, 1, 3, 2}
{2, 1, 3, 2}
lateVolumes = {volume[cu], volume[ag], volume[au], volume[zn]};
lateXAreas = {xArea[cu], xArea[ag], xArea[au], xArea[zn]};
lateMasses = {mass[cu], mass[ag], mass[au], mass[zn]};
```

lateVElectrons = {vElectrons[cu], vElectrons[ag], vElectrons[au], vElectrons[zn]};

```
lateTransitionWeightedVolume = Quiet|
    Total[lateVolumes[#] * lateFeatures[#] & /@ Range[1, Length[lateFeatures]], {1}] /.
                                   lateTransitionTotal
   {Indeterminate → 0};
lateTransitionWeightedArea =
        Total[lateXAreas[#] * lateFeatures[#] & /@ Range[1, Length[lateFeatures]], {1}]
                                       lateTransitionTotal
   {Indeterminate → 0};
lateTransitionWeightedMass =
  Quiet[ Total[lateMasses[#] * lateFeatures[#] & /@ Range[1, Length[lateFeatures]], {1}] /.
                                      lateTransitionTotal
   {Indeterminate → 0};
lateTransitionMeanVElectrons = Quiet[
    Total[N@lateVElectrons[#] * lateFeatures[#] & /@Range[1, Length[lateFeatures]], {1}]
                                     lateTransitionTotal
    /. {Indeterminate → 0};
Early Transition Transforms
earlyVolumes = {volume[ti], volume[v], volume[cr], volume[zr], volume[nb], volume[mo],
   volume[hf], volume[ta], volume[w], volume[ce], volume[pr], volume[gd], volume[u]);
earlyXAreas = {xArea[ti], xArea[v], xArea[cr], xArea[zr], xArea[nb], xArea[mo],
   xArea[hf], xArea[ta], xArea[w], xArea[ce], xArea[pr], xArea[gd], xArea[u]};
earlyMasses = {mass[ti], mass[v], mass[cr], mass[zr], mass[nb], mass[mo],
   mass[hf], mass[ta], mass[w], mass[ce], mass[pr], mass[gd], mass[u]);
earlyVElectrons = {vElectrons[ti], vElectrons[v], vElectrons[cr], vElectrons[zr],
   vElectrons[nb], vElectrons[mo], vElectrons[hf], vElectrons[ta], vElectrons[w],
   vElectrons[ce], vElectrons[pr], vElectrons[gd], vElectrons[u]};
earlyTransitionWeightedVolume = Quiet[
    Total[earlyVolumes[#]] * earlyFeatures[#]] & /@ Range[1, Length[earlyFeatures]], {1}] /.
                                   earlyTransitionTotal
   {Indeterminate → 0};
earlyTransitionWeightedArea = Quiet[
    Total[earlyXAreas[#] * earlyFeatures[#] & /@ Range[1, Length[earlyFeatures]], {1}] /.
                                   earlyTransitionTotal
   {Indeterminate → 0};
earlyTransitionWeightedMass = Quiet |
    \frac{\texttt{Total[earlyMasses[\#]} * earlyFeatures[\#] \& /@ Range[1, Length[earlyFeatures]], \{1\}]}{}] /.
                                   earlyTransitionTotal
   {Indeterminate → 0};
earlyTransitionMeanVElectrons =
  Quiet [ Total [N@earlyVElectrons [#]] * earlyFeatures [#]] & /@earlyTransitionTotal
        Range[1, Length[earlyFeatures]], {1}]] /. {Indeterminate → 0};
```

Temperature Differences

```
deltaT0 = annealingTemp - primaryCrystalOnset /. ___ - _ → "";
deltaT1 = annealingTemp - primaryCrystalPeak /. ___ - _ → "";
deltaT2 = annealingTemp - secondaryCrystalPeak /. ___ - _ → "";
```

Element Identity String

elementFeatures = {percentFe, percentSi, percentC, percentAl, percentB, percentP, percentGa, percentGe, lateTransitionTotal, earlyTransitionTotal}

```
{····1····}
                                               show all
                                                            set size limit...
large output
                show less
                               show more
```

compRows = Transpose[elementFeatures]

```
\{72.5, 13.5, 0, 0, 9, 0, 0, 1, 1, 3\}, \{71.5, 9.5, 0, 1, 9, 0, 0, 5, 1, 3\},
 \{73.5, 13.5, 0, 0, 9, 0, 0, 0, 1, 3\}, \{73.5, 13.5, 0, 0, 9, 0, 0, 0, 1, 3\},
 \{73.5, 13.5, 0, 0, 7, 0, 0, 2, 1, 3\}, \dots 1284 \dots, \{81, 4, 0, 0, 13, 0, 0, 0, 2, 0\},
 \{81.3, 4, 0, 0, 13, 0, 0, 0, 1.7, 0\}, \{81.3, 4, 0, 0, 13, 0, 0, 0, 1.7, 0\},
 \{81.3, 4, 0, 0, 13, 0, 0, 0, 1.7, 0\}, \{81, 4, 0, 0, 13, 0, 0, 0, 2, 0\}
large output
               show less
                             show more
                                            show all
                                                        set size limit...
```

```
isPresent[amount_] := { "0" amount == 0
    "1" amount ≠ 0
compID[elements_] := Module[
  {compstring = ""},
  For[
   i = 1, i ≤ Length[elements], i++,
   compstring = compstring <> isPresent[elements[i]]
  ];
  compstring
compIDColumn = compID[#] & /@ compRows;
```

New Data Set

```
newLabels = {"Total SiCAl", "Total BP", "Total GaGe",
   "Total Late Transition", "Total Early Transition", "Relative to Fe SiCAl",
   "Relative to Fe BP", "Relative to Fe GaGe", "Relative to Fe Early",
   "Relative to Fe Late", "Relative to Late Early", "Relative to Early SiCAl",
   "Relative to Late SiCAl", "Relative to Early BP", "Relative to Late BP",
   "Relative to Early GaGe", "Relative to Late GaGe", "Late Weighted Volume",
   "Late Weighted Area", "Late Weighted Mass", "Late Mean Electrons",
   "Early Weighted Volume", "Early Weighted Area", "Early Weighted Mass",
   "Early Mean Electrons", "Delta T0", "Delta T1", "Delta T2"};
allLabels = Join[newLabels, rawLabels];
newFeatures = {percentSiCAl, percentBP, percentGaGe, lateTransitionTotal,
   earlyTransitionTotal, relativeToFeSiCAl, relativeToFeBP, relativeToFeGaGe,
   relativeToFeEarlyTransition, relativeToFeLateTransition, relativeToLateEarly,
   relativeToEarlySiCAl, relativeToLateSiCAl, relativeToEarlyBP, relativeToLateBP,
   relativeToEarlyGaGe, relativeToLateGaGe, lateTransitionWeightedVolume,
   lateTransitionWeightedArea, lateTransitionWeightedMass, lateTransitionMeanVElectrons,
   earlyTransitionWeightedVolume, earlyTransitionWeightedArea,
   earlyTransitionWeightedMass, earlyTransitionMeanVElectrons, deltaT0, deltaT1, deltaT2};
allFeatures = Join[newFeatures, rawFeatures];
targets = {{coercivity, "Coercivity"}, {curieTemp, "Curie Temp"},
   {coreLoss, "Core Loss"}, {electricalResistivity, "Electrical Resistivity"},
   {permeability, "Permeability"}, {magnetostriction, "Magnetostriction"},
   {magneticSaturation, "Magnetic Saturation"}, {grainDiameter, "Grain Diameter"},
   {compIDColumn, "Composition ID"}, {doi, "Reference DOI"}};
masterDataset =
 Prepend[Transpose[Join[allFeatures, targets[All, 1]]], Join[allLabels, targets[All, 2]]]
Export["MasterDataset7-26.csv", masterDataset]
  {f Total SiCAl, Total BP, Total GaGe, Total Late Transition, Total Early Transition, }
    Relative to Fe SiCAl, Relative to Fe BP, Relative to Fe GaGe, ....55..., Core Loss,
    Electrical Resistivity, Permeability, Magnetostriction, Magnetic Saturation,
    Grain Diameter, Composition ID, Reference DOI \, . ...1293 ..., \ ( ... 1 ... ) \
 large output
               show less
                           show more
                                        show all
                                                  set size limit...
MasterDataset7-26.csv
(*fullFeatureDataSet[{target_,label_}]:=
 Prepend[Transpose[Join[allFeatures, {target}]], Join[allLabels, {label}]]
   newFeatureDataSet[{target_,label_}]:=
  Prepend[Transpose[Join[newFeatures, {target}]], Join[newLabels, {label}]]
    rawFeatureDataSet[{target_,label_}]:=
   Prepend[Transpose[Join[rawFeatures, {target}]], Join[rawLabels, {label}]] *)
```

```
(*fullFeatureDataSets=fullFeatureDataSet[#]&/@targets;
newFeatureDataSets=newFeatureDataSet[#]&/@targets;
rawFeatureDataSets=rawFeatureDataSet[#]&/@targets;*)
(*Export["FullFeatureCoercivity.csv",fullFeatureDataSets[1]]
Export["FullFeatureCurieTemp.csv",fullFeatureDataSets[2]]
Export["FullFeatureCoreLoss.csv",fullFeatureDataSets[3]]
Export["FullFeatureElectricalResistivity.csv",fullFeatureDataSets[4]]]
Export["FullFeaturePermeability.csv",fullFeatureDataSets[5]]
Export["FullFeatureMagnetostriction.csv",fullFeatureDataSets[6]]
Export["FullFeatureMagneticSaturation.csv",fullFeatureDataSets[7]]
Export["FullFeatureGrainDiameter.csv",fullFeatureDataSets[8]]
Export["FullFeatureLatticeParameter.csv",fullFeatureDataSets[[9]]]*)
(*Export["NewFeatureCoercivity.csv",newFeatureDataSets[1]]]
Export["NewFeatureCurieTemp.csv", newFeatureDataSets[2]]
Export ["NewFeatureCoreLoss.csv", newFeatureDataSets[[3]]]
Export["NewFeatureElectricalResistivity.csv",newFeatureDataSets[[4]]]
Export["NewFeaturePermeability.csv", newFeatureDataSets[5]]
Export["NewFeatureMagnetostriction.csv", newFeatureDataSets[6]]]
Export["NewFeatureMagneticSaturation.csv",newFeatureDataSets[7]]]
Export["NewFeatureGrainDiameter.csv",newFeatureDataSets[8]]
Export["NewFeatureLatticeParameter.csv",newFeatureDataSets[9]]*)
(*Export["RawFeatureCoercivity.csv",rawFeatureDataSets[1]]
Export["RawFeatureCurieTemp.csv",rawFeatureDataSets[2]]
Export["RawFeatureCoreLoss.csv", rawFeatureDataSets[3]]]
Export["RawFeatureElectricalResistivity.csv",rawFeatureDataSets[[4]]]
Export["RawFeaturePermeability.csv", rawFeatureDataSets[5]]]
Export["RawFeatureMagnetostriction.csv", rawFeatureDataSets[6]]
Export["RawFeatureMagneticSaturation.csv",rawFeatureDataSets[7]]]
Export["RawFeatureGrainDiameter.csv", rawFeatureDataSets[8]]
Export["RawFeatureLatticeParameter.csv",rawFeatureDataSets[[9]]]*)
```