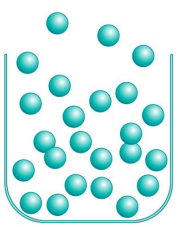
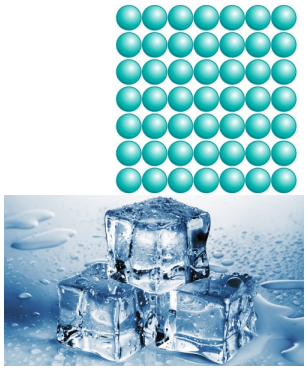
4.相，点缺陷，合金固溶体

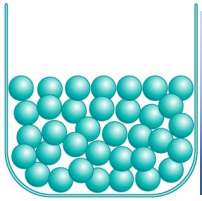
Dongsheng Wen

相 (phase)

- 定义







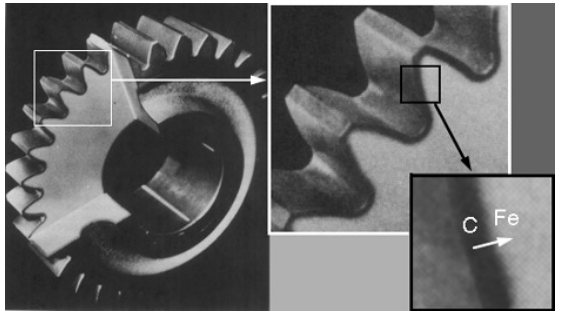
相：生活中的例子

气相

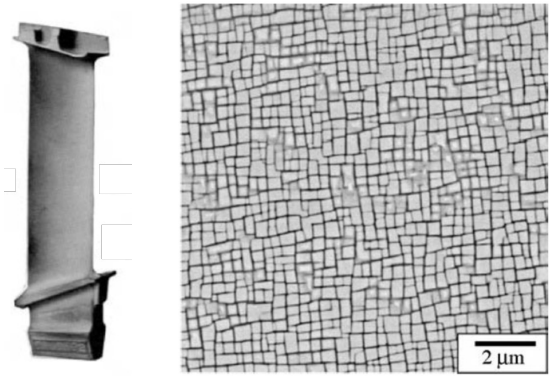
液相

Martin Leigh / Getty Images

固相



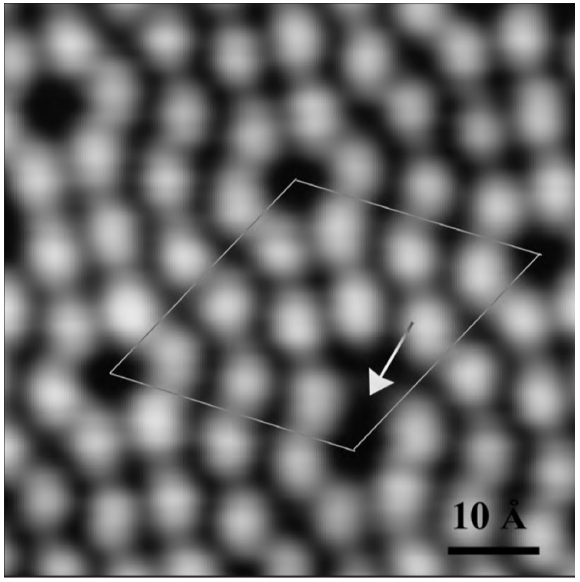
http://www.rkriz.net/sv/classes/MSE2094_NoteBook/96ClassProj/examples/charcon.html

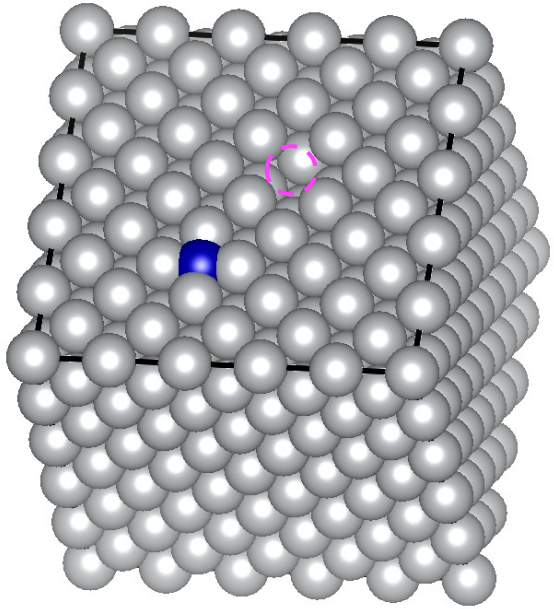


The Superalloys Fundamentals and Applications, Roger C. Reed

完美的材料是不存在的！！！

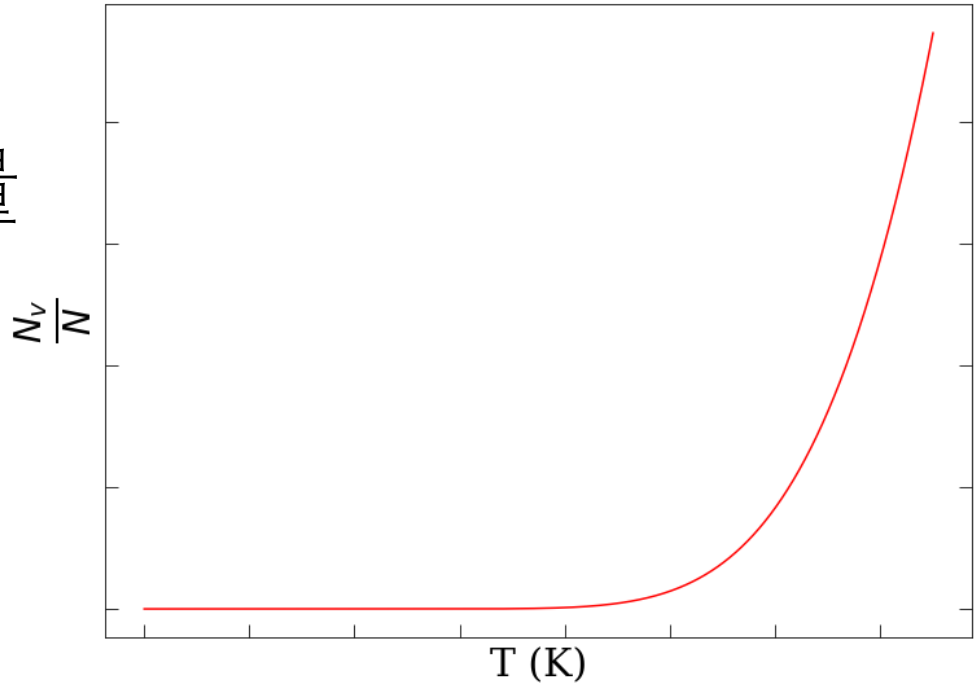
- 缺陷 (defects)的一种：点缺陷 (point defect)





空位 (vacancy)的数量

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$



- Cu的空位形成能$Q_v = 0.9eV/atom$, 求一小块 1 cm³ 的Cu在1000˚C时候的空位个数。
  - Cu的原子质量：63.5 g/mol
  - Cu的密度：8.4 g/cm²
  - $N_A = 6.023\times10^{23}$ atom/mol
  - $k = 8.62\times10^{-5}$ eV/K/atom

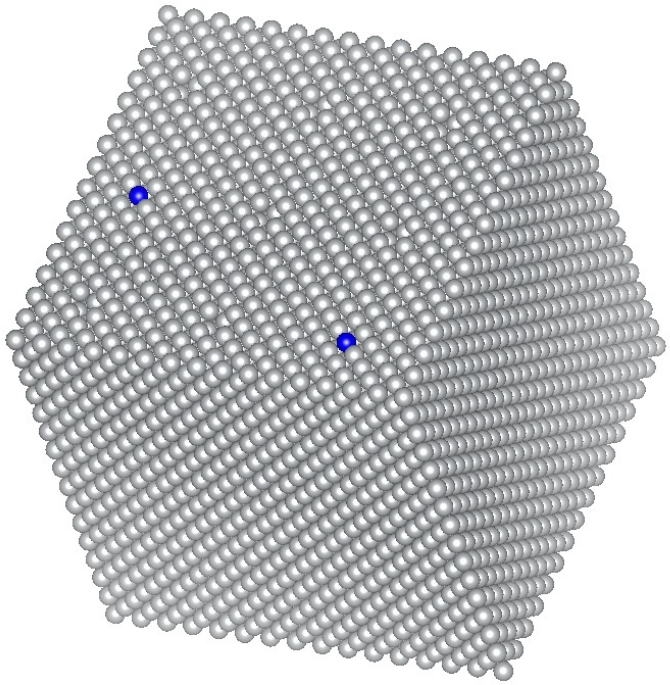
100%纯的材料也是不可能的！！！

- 原材料市场上可以买到的高纯度金属：
- 纯镍 Ni

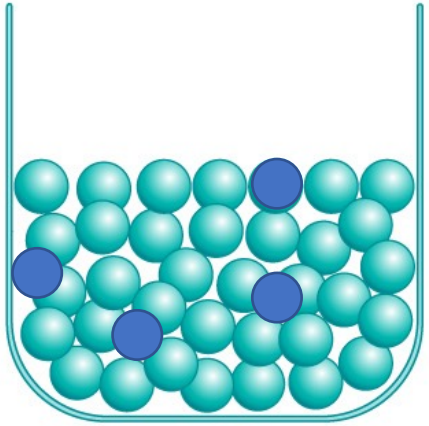
http://www.goodfellow.com/catalogue/GFCat4.php?ewd_token=Ov790HvMN084SAaInHReLpY3iES3nc&n=mfFmAKLQ5nI5KAtuZmiMIfeiLw5bwE

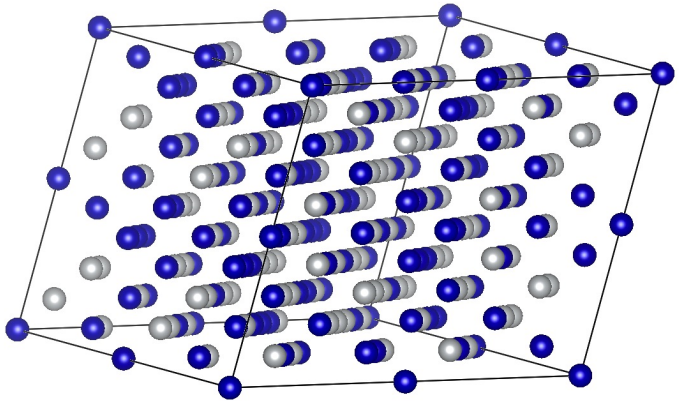
819-960-14	99.99%	100 g	USD 504.00
567-913-78	99.999%	100 g	USD 1111.00

- 杂质原子:

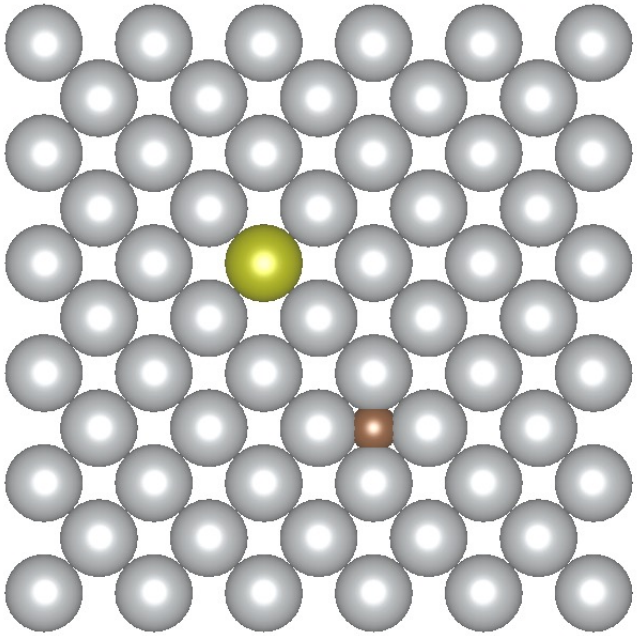


合金结构





- 固溶体 (solid solution)
  - 溶剂原子
  - 溶质原子
  - 成分

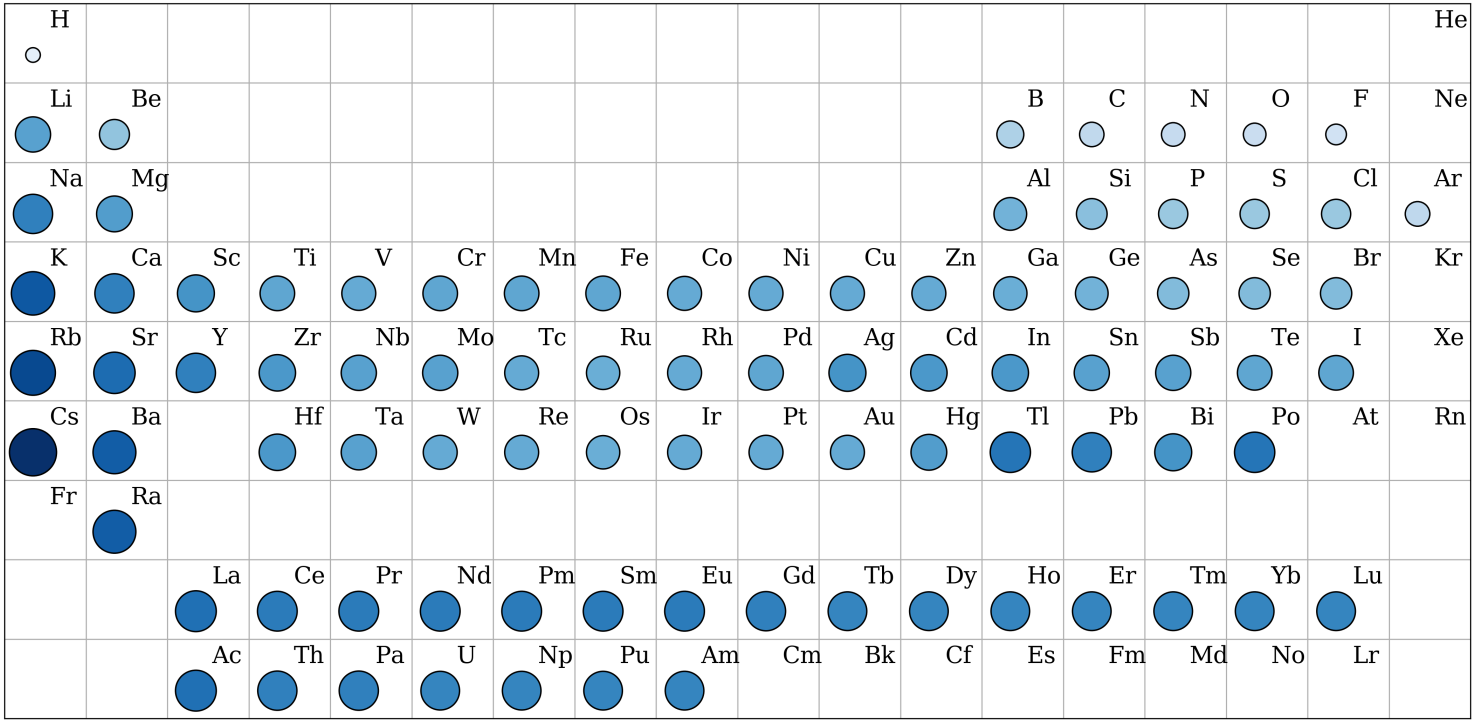


- 置换固溶体 (substitutional solid solution)
- 间隙固溶体 (interstitial solid solution)

什么影响了固溶体形成？

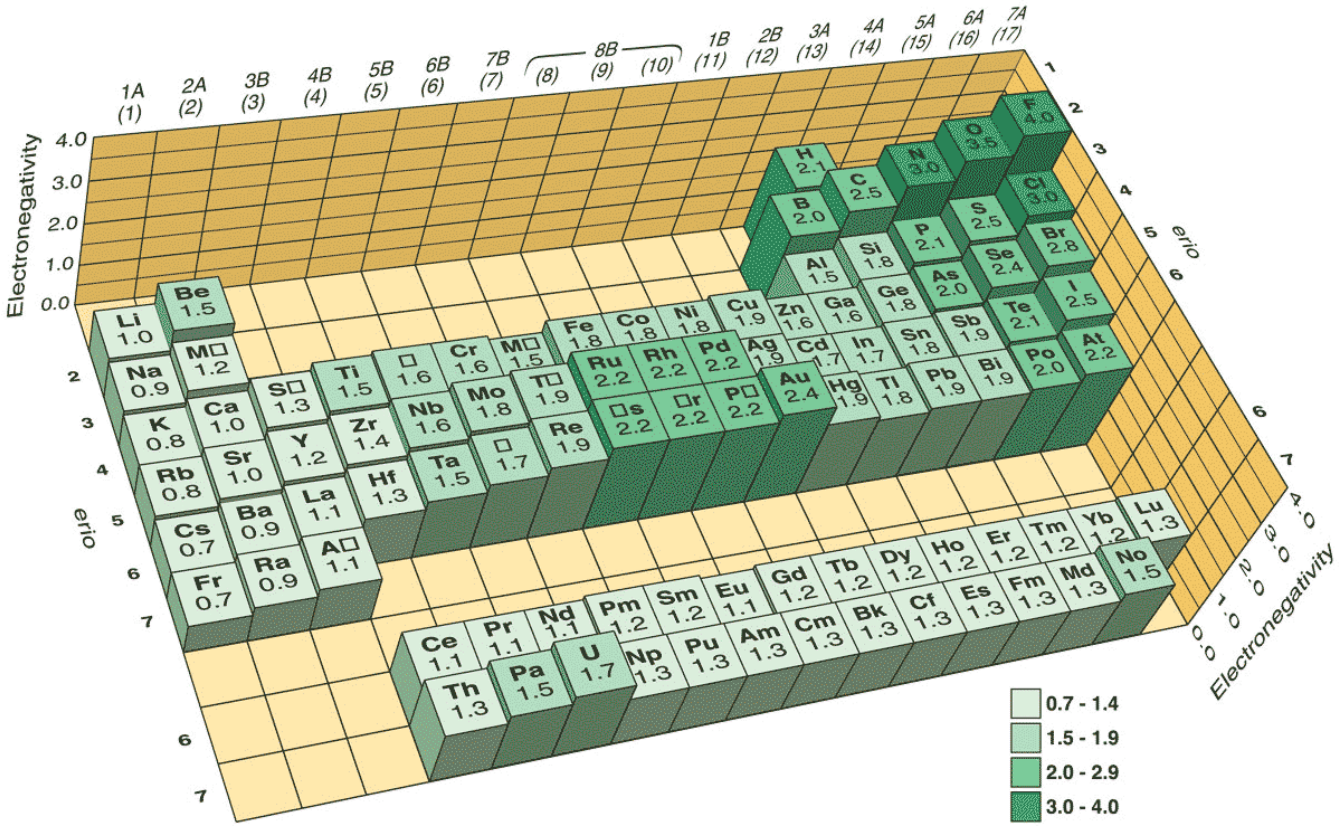
- 原子尺寸因素 (atom size factor)
- 晶体结构 (crystal structure)
- 电负性 (electronegativity)
- 原子价 (valences)

原子尺寸因素和晶体结构



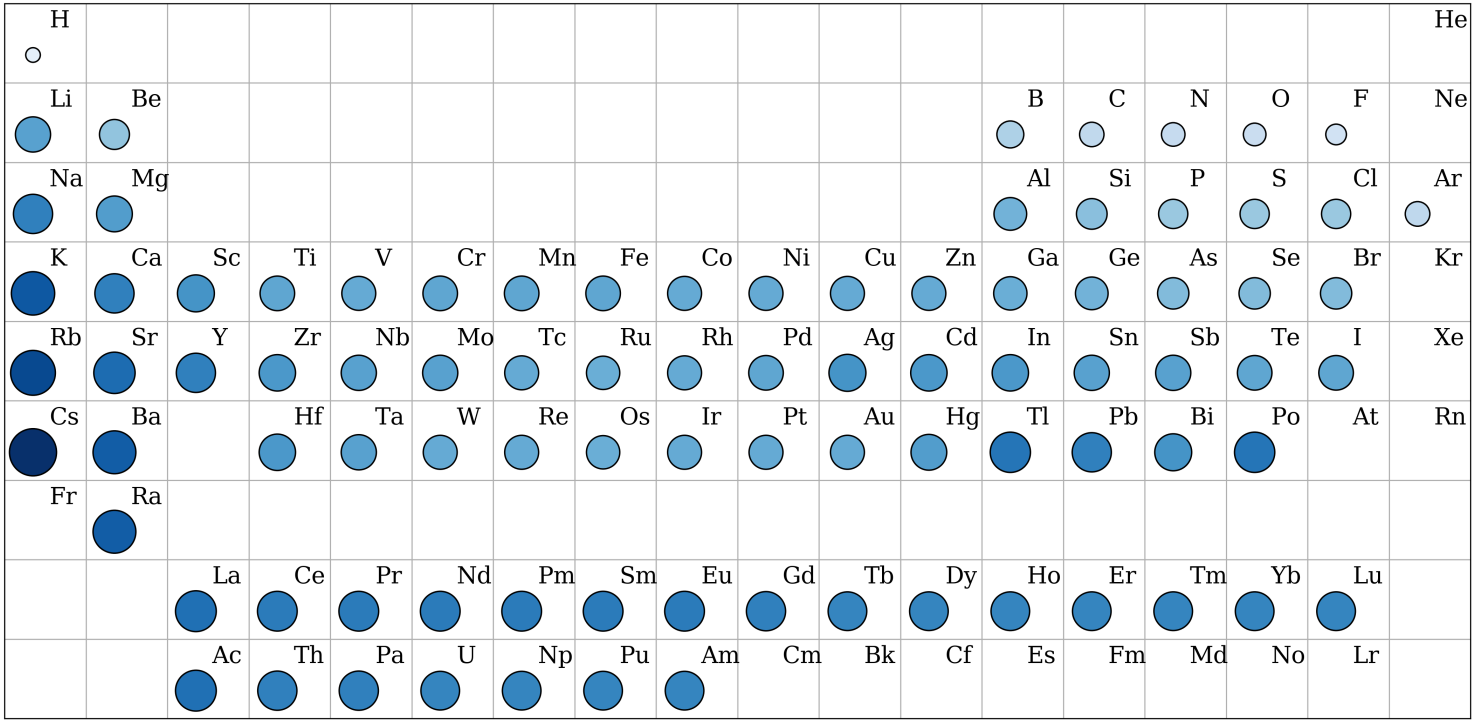
数据来源：pymatgen

电负性



https://derekcarrsavvy-chemist.blogspot.ca/2016/01/periodicity-1-ionisation-energy-and.html

原子价


H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

5.力学性能测试，应力/应变

dswen94