First principles calculations of solute atoms in bcc-Fe

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The solute atoms in matrix alloys affects the mechanical properties via lattice distortion. Especially on bcc-Fe, the small amounts of solute atoms control the matrix hardening or elongation, which plays main role on the industrial materials. Atomic radii for pure metals and diluted alloys in Fe show similar trends on periodic table as shown in Fig. 1. At every row of the periodic table, the radii show minima at close to the same group of Fe, but bigger deviation at stepping away at both ends.

For this research, we will give the first principles calculations of dilute atoms from Ti to Zn in bcc-Fe. Using VASP code, the energy-volume curves for pure metals and model lattice of dilution alloys are obtained. The radii of pure metals with bcc lattice and diluted metal in bcc-Fe are calculated from these curves.

Calculated results are shown in Fig. 2. Early transition metals show very similar trends between the calculated and experimental results for both pure metal with bcc structure and effective radius of metal diluted in bcc-Fe. But for the late transition metals of Cu, Zn, the trends are slightly deviated from the experimental results. Overall trend will be explained from the binding behaviour of dilute atoms with bcc-Fe. The hardness, which is given by the second derivatives of energy-volume curve, also shows the similar behaviour rooted in the same origin.