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The effect of temperature on the calculated bulk vacancy formation energy in Al and Cu

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Abstract content
   (Max 300 words)

1. Abstract

The vacancy formation energy is an important factor in diffusion kinetics, and has been shown to be dependent on surface orientation in both Al and Cu.1,2 What has not yet been extensively studied is the effect of temperature on these vacancy formation energies, but with the use of density functional theory (DFT) it has been shown for Pt, Pd and Mo that the vacancy formation energy increases with temperature.3 Perfect crystals of Al and Cu were simulated with the use of an embedded atom potential developed by Sutton and Chen.4 The crystals were simulated with surface orientations of (100), (110) and (111) at a range of temperatures. The vacancy formation energy was obtained by finding the difference between the energy needed to remove an atom from inside the crystal volume and the energy obtained from adding an atom to the crystal surface.1,2,5 Bulk binding energies were largely unaffected by the change in temperature, thus the temperature dependence of the average surface binding energies were measured for the points most likely to bond an atom on the surface. Using likely bonding sites, the average surface binding energy f or each crystal was determined for various temperatures. The binding energies were monitored over time to ensure a good average of the surface binding energy for each temperature.

1. References

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