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The calculated vacancy formation energies of Al, Ni, Cu, Pd, Ag, and Pt.

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Abstract content
   (Max 300 words)

A molecular dynamics simulation that made use of the Sutton-Chen many-body potential [1] calculated the bulk vacancy formation energies (Ev) for Al, Ni, Cu, Pd, Ag, and Pt single crystals. The Ev values for single crystals with the surface orientations of (111), (100) and (110) were calculated at temperatures ranging from 0 K to 1000 K. In the case of Cu and Al which showed premelting below 1000 K, Ev values were calculated up to below their respective premelting temperatures. The values obtained for vacancy formation energies at 0 K exhibited surface orientation dependence and compared well to values obtained from literature. [2-4] The (111) surface had the closest packed surface, with few atoms bonding to a surface adatom, and had the highest bulk vacancy formation energy. The (100) surface had average Ev values that compare well with surface-independent literature values. [4] The (110) surface had deep surface binding sites with the largest number of surface atoms able to bond to an adatom and had the lowest bulk vacancy formation energy. For an increase in temperature a slight decreasing trend in Ev values was observed, which is associated with atoms in the bulk that bond less strongly as a result of the crystal expansion at higher temperatures. Disordering was observed at temperatures well below the melting points of Al, Cu, Ag and Ni. At these temperatures where surface disordering occurred in (110), surface instability interfered with deep binding sites on the surface, reflected in a slight increase in Ev values. Disordering occurring in (111) and (100) surface orientations at high temperatures conversely allowed deeper binding sites in the tightly packed surfaces and resulted in a slight drop in Ev values.

References
[1] Sutton, A. P.; Chen, J., Phil. Mag. Lett., 1990, 61, 139-146.
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[3] Terblans, J. J. Surf. Interface Anal. 2003, 35, 548–551.
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Primary author: Ms VAN DER WALT, Cornelia (Physics Department, University of the Free State)

Co-authors: Prof. SWART, Hendrik (Physics Department, University of the Free State); Prof. TERBLANS, Koos (Physics Department, University of the Free State)

Presenter: Ms VAN DER WALT, Cornelia (Physics Department, University of the Free State)

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