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Trapping of He clusters by inert-gas impurities in refractory bcc transition metals: systematic first-principles predictions and experimental validation

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Recently, systematic quantum-mechanical calculations of radiation defects in tungsten and iron-based alloys play important role in understanding generic materials-related problems foreseen with operation of future fusion-power plants [1-5]. In this talk, properties of point defects resulting from the incorporation of inert-gas atoms in bcc transition metals (TMs) are investigated systematically using first-principles density functional theory (DFT) calculations. For the TMs in group 6B (Cr, Mo, W) of periodic table and Fe, the most stable configuration for the interstitial neon, argon, krypton and xenon atoms is predicted in the tetrahedral site, similarly to what was found earlier for helium in all bcc TMs, whereas for the TMs in group 5B (V, Nb, Ta) the octahedral configuration is the most energetically favourable one. The calculated formation energies for single inert-gas atoms at interstitial sites are systematically larger for Ne, Ar, Kr and Xe than for the case of He and this trend can be simply understood by a strong local distortion with respect to their atomic size. However, a deeper analysis their substitutional formation energies demonstrates that vacancy-impurity interaction is more likely to be related to the covalent character of bonding between inert-gas atoms and bcc TMs. There is a remarkable variation exhibited by the binding energy between inert-gas impurity and vacancy going from He to Ne, Ar, Kr, Xe. The origin of this trend is explained by electronic structure calculations showing that *p*-orbitals play an important part in the formation of chemical bonds between a vacancy and an atom of any of the four inert-gas elements in comparison with helium, where the latter contains only $1s^2$ electrons in the outer shell. The binding energies of a helium atom trapped by five different defects (He-v, Ne-v, Ar-v, Kr-v, Xe-v, where v denotes a vacancy) are all in excellent agreement with experimental data derived from thermal desorption spectroscopy (TDS) for bcc-W. Attachment of He clusters to inert gas impurity atom in all bcc TMs is analysed as a function of the number of successive helium atoms trapped in that created by the prior inert-gas heavy ion bombardment with several discrete binding energies measured within the TDS experiments [6]. The present DFT data base can be used to explain the swelling and variation of the Young modulus due to inert-gas ion implantation in plasma facing materials for fusion device applications [7].

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