INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Inert-gas defects in bcc transition metals: Systematic trends and experimental validations

One of the main objectives for the EFDA materials modelling and experimental validation program is to develop an accurate predictive model for defects formed due to the accumulation of helium and other inert gases in the crystal lattice of iron, steels and non-magnetic bodycentered cubic (bcc) refractory metals, and to offer a way of quantifying the effect of damages induced by ion-beam irradiation on the structural integrity of reactor components.

We have carried out a systematic study of defects, resulting from the incorporation of noble-gas atoms (He, Ne, Ar, Kr, Xe) into all the bcc transition metals, including iron, using first principles density functional theory (DFT) calculations. The formation energies of various substitutional and interstitial configurations of noble-gas atoms have been calculated to understand the trends and to quantify the local lattice distortion effects as a function of the noble-gas atom size. Helium is a relatively small atom and He defect energies are lower than those corresponding to other noble gas atoms. The size effect results in the change of the relative stability of tetrahedral and octahedral interstitial sites for Ne, Ar, Kr and Xe in comparison with He. A remarkable attractive binding energy trend involving interaction between inert-gas atoms and vacancies is systematically investigated, showing a pronounced and colossal size effect going from He to Ne, Ar, Kr, Xe. Interestingly, the origin of this systematic trend can be revealed by electronic structure calculations from which the p-orbitals play an important role for distinguishing the latter four inert-gas elements in a comparison with helium with only 1s2 electrons in the outermost shell. The present DFT predicted trends have been validated by experimental measurements from thermal desorption spectroscopy of helium atom trapped by five impurities (the substitution He atom He, Ne, Ar, Kr, Xe) in tungsten. Our DFT data base is also being used for understanding swelling properties of bcc transition metal under inert-gas ion implantation. Finally systematic trends of incorporation energy for He and other inert gas atoms in all bcc transition metals are employed to re-evaluating the life-time of components of fusion power plant within an integrated model.

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