Nanoobjects microscopy

Interaction energy of self-interstitial atoms with grain boundaries in tungsten

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The energetics of SIAs interacting with high-angle GBs in tungsten were investigated "in situ" during irradiation with 5 keV He atoms at fluences of 10^{16} – 10^{17} atoms/m^2 by field ion microscopy (FIM). This FIM technique with the field evaporation phenomenon were used to find the formation energy of self-interstitial atoms at GBs in tungsten.

It was shown earlier that during SIA emergence on the free surface the potential energy of their implantation transforms into surface atom kinetic energy. The magnitude of this excitation can be determined by [1]. The method for SIA formation energy determination is based on a quite strong dependence of the threshold field for evaporation on the total energy of the surface atoms described by the "image hump" theory. Cases of SIA emerging into surface through grain boundaries and through crystalline bulk were studied separately. The SIA binding energy, which is equal to SIA interaction energy, was calculated as the difference between the SIA formation energy in a monocrystal and in a GB.

It was found that the energy distribution is characterized by a broad spectrum from 0.50 to 5.0 eV with a full width at half maximum of 1.98eV and with the peak at 2.89 eV [2]. Variations in SIA formation energy in GBs indicate to huge diversity of positions in GBs that SIA can occupy. The obtained result can point to low SIA mobility along GBs.

1. *I.M. Neklyudov,E.V.Sadanov,G.D.Tolstolutskaja,V.A.Ksenofontov,T.I. Mazilova,I.M.Mikhailovskij* Interstitial atoms in tungsten: Interaction with free surface and in situ determination of formation energy // Phys Rev B.-2008.-**78.**-115418

2. *E.V. Sadanov, O.V.Dudka, V.A.Ksenofontov, T.I.Mazilova, I.V.Starchenko, V.L. Manakin, I.M.Mikhailovskij* Binding energy of self-interstitial atoms to grain boundaries: An experimental approach // Mat Let.-2016.-**183.**-P. 139-142.