Nanoscale physics

Nanoscale modulated dissipative distributions of interacting vacancies within the irradiated b.c.c. crystal

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Within the crystals under irradiation, the modulated structures can be formed [1]. The report is concerned with study of conditions of self-organizing of a precursor of formation of a superlattice of nanovoids, namely, the modulated structure in distribution of the vacancies generated by an irradiation because of instability of their homogeneous distribution as a result of interaction between them within the cubic crystal, which is irradiated. For instance, with b.c.c. crystal as a model of the irradiated functional material, the numerical and analytical calculations of energy parameters for 'strain-induced' and 'electrochemical' interactions of vacancies within the b.c.c. crystal are carried out. Their behaviour near and far from the centre of the b.c.c.-lattice reciprocal-space Brillouin zone (particularly, on its surface) is studied. The temperature dependence of spatial period $d(T)$ of the modulated dissipative structure of vacancies' subsystem in b.c.c. crystal is numerically forecasted and analysed, taking into account the total ('electrochemical' + 'strain-induced') interaction between vacancies.

Temperature dependences of the periods of the modulated structures in distribution of vacancies and nanovoids are estimated. As shown, if density of dislocations is temperature independent, the period of the dissipative modulated structure in a spatial distribution of vacancies decreases slightly with temperature increasing and is conditioned by 'electrochemical' interaction of vacancies. Accounting (empirical) temperature dependence of density of dislocations leads to increasing the dissipative modulated structure period with temperature that is caused by the entropy factor and 'electrochemical' interaction of vacancies. The period of superlattice of nanovoids increases with temperature since it is determined only by their elastic interaction.

1. *Ghoniem N. M., Walgraef D., Zinkle S. J.* Theory and experiment of nanostructure self-organization in irradiated materials // J. Comput.-Aided Mol.

Des.-2002.-**8**.-P. 1-38.