QUANTUM BEHAVIOR OF THE STACKING FAULTS (SF) IN hcp CRYSTALS OF HELIUM

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The helium crystals can be as a convenient model object for the simulation of atomic crystals and study their quantum properties [1]. In solid helium the phase transition, the bcc-hcp coherent phase boundary (PB) and twin boundary (TB) were investigated theoretically in the frames of one order parameter (OP) model, the authors examined the behavior of the classical phase boundaries and domain walls in metals and helium, and their influence on the asymmetry of the phase transition. The two order parameters theory was developed on the base of the Burgers mechanism. Twin boundaries or domain walls (DW) are formed in processes of growth and deformation of the crystal. We proposed the three OP theory that combines Sanati and Kaschenko treatments that allows taking into account the changes in volume and pressure under the phase transition. We have shown that the three OP and one OP descriptions of PB and TB are uniquely associated.

In this report, the 180^{o} domain wall or the stacking fault (SF) are investigated in the hcp lattice. In SF the lattice potential for an atom reduces its symmetry and is elongated along the direction [2110] hcp of the shift of the atomic planes. We solve the problem of finding the wave function of the helium atom for (i) a spherical oscillator (within the hcp phase) and (ii) an anisotropic one (in DW). It is shown that the isosurfaces of the probability density are transformed from the spheres in the hcp phase into ellipsoids inside the DW. To estimate the parameters of the thermodynamic potential we apply the model of spheres and ellipsoids. Method of the successive approximations is applied for the self-consistent description of the deformation of the wave function of atoms. Consequences of the quantum behavior of the crystal in SF are follows: (i) increasing of the degree of overlap of atomic wave functions within SF, (ii) the resulting increase in the quantum diffusion of SF, (iii) reduction of energy and an increase in thickness of the wall in comparison with the classical case.

Literature:

1. Manzheliĭ V. G. Physics of Cryocrystals / V. G. Manzheliĭ and Y. A. Freiman. – NY: Woodbury, AIP – P.691.