Effect of the thermal vibration on the acceleration of neutral atoms during a surface phase transition

I.Yu. Goliney, V.V. Mykhaylovskyy and V.I. Sugakov

Institute for Nuclear Research, Nat. Acad. Sci. of Ukraine, 47 Prospekt Nauki, Kiev, Ukraine E–mail: igoliney@kinr.kiev.ua

The paper explores the possibility and criteria for the acceleration of neutral atoms during phase transitions at the crystal surfaces. It continues similar studies performed for bulk crystals.

The acceleration occurs via a sequence of consecutive atomic collisions during which an atom in the metastable state transfers to a new stable position giving its excess energy to the next atom in the row. The chain of collision may occur coherently and involve a significant number of atoms enabling the last atom in the chain to harvest considerable energy.

The paper considers a phase transition in the system of adatoms at the crystal surface with a filling factor of 1/4. The adatoms, weakly interacting with the surface and being attracted to the sites of the square lattice of the substrate and strongly interacting with each other, may form two types of lattices at the surface: a square lattice and a rectangular base centered lattice. The phase transition between the lattices happens with changing the lattice constant of the substrate.

The acceleration of atoms was confirmed by the methods of molecular dynamics. The largest velocity of the accelerated atoms for different temperatures was determined. The energy of the accelerated atoms is of order of several tens of eV exceeding by much the thermal energy. Additionally to the single atom acceleration a regime in which two atoms were accelerated was observed. Different processes that require a considerable activation energy usually unavailable trough thermal excitations may be facilitated by the emergence of such accelerated atoms during phase transitions. The process that belong to this class are the excitation of the high energy electronic levels with the emission in UV or X-ray ranges, stimulation of the nuclear reactions, etc.