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SESSION 1: MODELS AND METHODS, SALON A

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Molecular dynamics study of growth of silicon from melt and formation of dislocation

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ABSTRACT

Molecular dynamics simulations of growths of silicon crystalline from the melt along <111>, <100>, <110>, and <112> directions have been carried out. Tersoff potential is employed for computing atomic interaction. The results show that,

1. Anisotropic growth of silicon existed in the four directions of Si crystalline, and the sequence of growth rate is. The atomic distributions and diffusion coefficients affecting by the crystal orientations is the key factor of the anisotropic growth of silicon.
2. The formation of dislocations showed anisotropic laws. No dislocation was formed in the growths along <100> and <110>, while more than one dislocation formed along <112 and <111>. The dislocation formed is identified as a partial dislocation lying on an {111} plane, with segments of 30°partial dislocation, 90°partial dislocations, and some kinks. The dislocation nucleates stochastically at the crystal–melt interface, originated from at least two units of stable periodic non-six-member-ring groups.
3. Dislocations will furthermore affect the morphology of crystal–melt interface and the crystal growth rate. With an edge threading dislocation or dislocation-free, the (110) interface keeps zigzag morphology and continuous growth mechanism. However, with a screw threading dislocation, the interface contains a type of “V” groove around the outcrop of the dislocation and keeps a spiral growth mechanism. The screw dislocation prevents the crystal growth of Si, while the edge dislocation has a little influence on the crystal growth rate.

KEYWORDS: crystal growth from melt, anisotropic growth, dislocation, interface morphology, growth rate