

Abstract Submitted
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Dislocation nucleation in Si – effect of Ge and vacancies ZHI LI, CATALIN PICU, Rensselaer Polytechnic Institute — The presence of dislocations in Si devices is detrimental for their function. However, dislocations may nucleate during device processing from interfaces and from imperfections of the surface. In this work we study the conditions under which this may take place. Specifically, the activation energy for dislocation nucleation in pure Si is evaluated using an atomistic model and considering a corner stress concentrator. At lower temperatures, 60° dislocations nucleate in the shuffle set as half-hexagonal loops. The activation energy depends on the step height and on the spacing between steps. The effect of Ge on nucleation is evaluated using the same model and it is observed that the energy barrier decreases slightly in presence of these substitutional atoms. The presence of vacancies in the glide plane also decreases the activation energy. A low concentration of vacancies (0.5%) decreases the barrier for nucleation similarly with a large concentration of Ge (30%).

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