

Abstract Submitted
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Investigation of the structure and properties of vacancies in Si and Ge nano-crystals by *ab initio* methods¹ SCOTT BECKMAN, JAMES CHELIKOWSKY, University of Texas — The production of nano-scale devices requires the ability to selectively dope nano-structures either n-type or p-type. The functionality of such devices demands that the dopant species remains in the nano-structure, and not diffuse into neighboring regions or to surfaces. The diffusivity of impurities in a crystal depends explicitly upon the self-diffusion of the host species. Understanding this requires understanding the modes of self-diffusion, and the mobility of intrinsic defects in the host crystal. Here we investigate the structure and properties of vacancies in Si and Ge nano-crystals. Using a real space pseudopotential method we study the energy of vacancies within 2 nm diameter crystals. It is observed that vacancies are naturally pulled toward the surfaces; however, in highly symmetric crystals, it is possible to trap vacancies in the center of the crystal. Once a vacancy is within 0.4 nm of the surface a bucking effect occurs, which indicates that a surface reaction will probably act to pull the vacancy to the surface.

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