564d Defect Nucleation and Growth in Crystalline Silicon under Conditions of Generalized External Stress

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There is currently much interest in the use of lattice strain to tailor the atomic and electronic properties of hard semiconductor materials, such as silicon and silicon-germanium. For example, strained silicon layers fabricated on compositionally graded SiGe substrates have been demonstrated to enhance electron and hole mobility in complementary metal-oxide semiconductor (CMOS) technology. Large stresses also can be present unintentionally in conventional silicon microelectronic device processing, for example, resulting from thermal expansion mismatches between different materials. Such effects become increasingly important as tolerances on microstructural evolution become more stringent and length scales shrink.

While there have been many theoretical studies of point defect properties in simple stress fields, defect clustering is not at all well understood in the presence of complex stress fields and high temperature. Part of the reason for this is that point defect clusters tend to be geometrically complex and can assume numerous different configurations, especially at elevated temperature. How this ensemble of configurations responds to lattice stress is entirely unknown and could have significant consequences on the evolution of atomic aggregation during processing.

In this study we investigate, using large-scale molecular dynamics, the nucleation and growth of point defect aggregates in crystalline silicon under a wide variety of externally imposed stress fields. The mechanical field conditions are imposed using the constant-NST ensemble where the stress state (S) is imposed using extended Parinello-Rahman molecular dynamics. A variety of fields are investigated for both both vacancy and self-interstitial aggregation, beginning with simple hydrostatic pressure (tension and compression) and increasing the complexity to include various types of shear. The aggregation dynamics and resulting cluster morphology are analyzed in the context of experimental data.