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HD-PIT SiGe Hexagonal Diamond Phase by nanoIndenTation

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Pressure-Induced Phase Transitions and Electronic Impact of Extended Defects in Germanium and Silicon

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Silicon (Si) and Germanium (Ge) exhibit multiple metastable phases that hold promise for advancing optoelectronic integration into Si-based technologies. Specifically, the hexagonal diamond (hd) phase of Ge possesses a direct band gap [1], making it highly desirable. These metastable phases can be synthesized from the stable diamond cubic (dc) phase through a series of pressure-induced phase transitions, as observed experimentally via nanoindentation.

Leveraging machine learning (ML) interatomic potentials, we conducted extensive Molecular Dynamics (MD) simulations of the nanoindentation process [2] (as shown in Fig. 1) to capture the atomistic mechanisms underlying these pressure-induced transitions. We developed a Ge-specific ML potential [3], revealing key nucleation events and the interplay between localized nucleation kinetics and complete phase transitions under pressure. This study extends another similar study on Si, where existing ML potentials have uncovered complex phase transformation pathways [4].

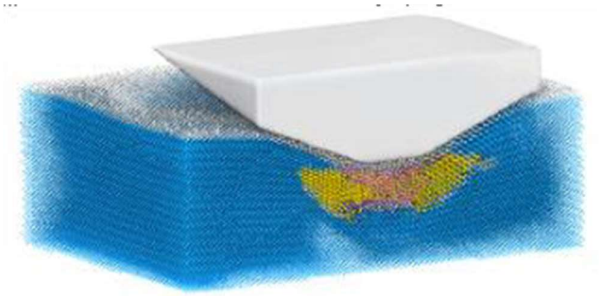

Figure 1: Large-scale MD simulation of the nanoindentation process. Several pressure-induced phase transitions strarting from the dc substrate (in blue in the figure) can be observed during the simulation and are highlighted in the figure by different colors.

To integrate these findings, we examined how extended defects such as dislocations and stacking faults, often formed during pressure-induced phase transformation or epitaxial growth of Ge on Si, influence its electronic properties. Ab initio calculations show that dislocations introduce electronic trap states in the band gap (see Fig.2), while stacking faults may lead to hexagonal inclusions that form Type-I quantum wells with a tunable direct band gap. These inclusions are predicted to induce a direct gap [5] consistent with recent experimental photoluminescence observations.

Our comprehensive approach, combining pressure-dependent phase transition analysis with electronic defect characterization, provides new insights into engineering the optoelectronic properties of group-IV semiconductors and suggests novel avenues for utilizing structural and electronic modifications of SiGe for future quantum and photonic technologies.

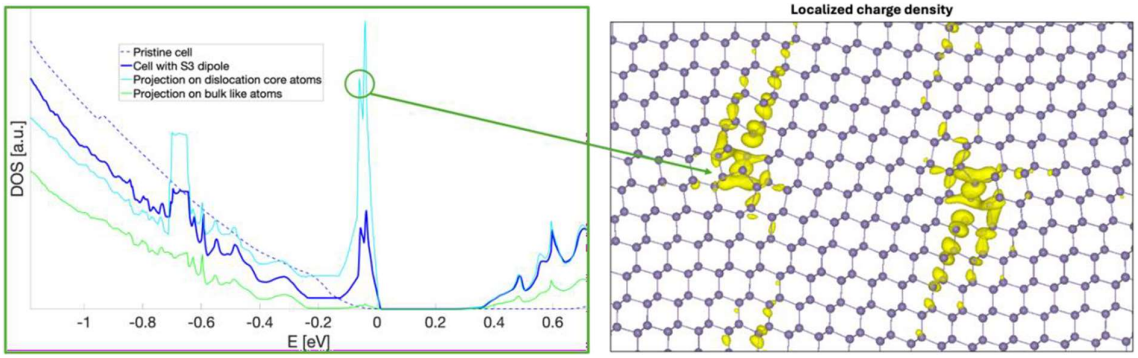

Figure 2: Electronic density of states of shuffle dislocation dipole in Ge. The real-space wavefunction (square) corresponding to an electronic state in the Ge bandgap is also shown, evidencing a charge density localized at the dislocation cores.

[1] E. Fadaly, *et al. Nature* **580**, 205–209 (2020)
[2] G. Ge, F. Rovaris *et al.* Acta Materialia **263**, 119465 (2024)
[3] A. Fantasia *et al.* JCP **161**, *014110* (2024)
[4] F. Rovaris *et al. Materials Today Nano (just accepted),* arXiv:2408.12358
[5] A. Marzegalli *et al.,* Nanoscale Horiz. **9**, 2320-2325 (2024)

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