Comparing the self-assembly of tensile-strained Ge and GaAs quantum dots on InAlAs(111)A

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 $2 \times 2 \mu m^2$ AFM images of tensilestrained (top) 0.6 BL Ge and (bottom) 4.5 ML GaAs QDs. We grew both samples at 535 °C. The top and bottom images have a zscalebar of 1.5 nm and 4 nm, respectively.

Compressively strained quantum dots (QDs) grown on (001) surfaces have been explored widely for optoelectronic applications. A recently developed process, tensile-strained self-assembly enables the tunable synthesis of defect-free QDs on non-(001) surfaces, opening up many potentially novel applications. For example, theory predicts that Ge will become a direct band gap semiconductor when grown on (110) surfaces under ~3% biaxial tensile strain and a semimetal on (111) surfaces under ~4% tensile strain.¹⁻⁴ (111)-oriented GaAs QDs are a promising source for entangled photons due to their high symmetry and low fine-structure splitting.

The development of tensile-strained self-assembly has chiefly focused on the growth of Ge and GaAs QDs on the (110) and (111)A surfaces of $In_{0.52}Al_{0.48}As$. With almost identical lattice constants, these Ge and GaAs QD systems are very similar from the point of view of tensile strain, with ~3.7% lattice mismatch. However, while exploring the self-assembly of tensile-strained Ge and GaAs QDs, we discovered significant differences between these two systems. Although both show excellent tunability in terms of QD size and areal density with growth conditions, Ge and GaAs QDs exhibit different shapes and nucleation behaviors. To understand these differences, we used a combination of experimental characterization and computational modelling. We compare experimentally derived island scaling and radial distribution functions to predictions from density functional theory and kinetic Monte Carlo simulations of potential energy surfaces (PES). We use this data to explore the

surface diffusion behavior of the Ge and Ga adatoms on InAs(111)A.

Under the same MBE growth conditions, Ge QDs have a higher critical cluster size than GaAs QDs, although in both cases these critical clusters seem to adopt a three-fold symmetry consistent with the (111)A surface. Our models indicate that the InAlAs surface has an As-trimer reconstruction, and preliminary results show marked differences in the migration behavior of Ge and Ga adatoms on this surface. The potential barriers to Ge adatom surface diffusion appear to be lower than for Ga adatoms, resulting in longer diffusion lengths. We will discuss our experimental and computational results from both a kinetic and thermodynamic perspective.

¹ H. Tahini, A. Chroneos, R.W. Grimes, U. Schwingenschlögl, and A. Dimoulas, J. Phys. Condens. Matter 24, 195802 (2012).

² O. Aldaghri, Z. Ikonić, and R.W. Kelsall, J. Appl. Phys. **111**, 53106 (2012).

³ H.S. Lan, S.T. Chan, T.H. Cheng, C.Y. Chen, S.R. Jan, and C.W. Liu, Appl. Phys. Lett. 98, 101106 (2011).

⁴ M. El Kurdi, G. Fishman, S. Sauvage, and P. Boucaud, J. Appl. Phys. **107**, 13710 (2010).



Fig. 1. As-trimer PES for a Ge adatom on In(Al)As(111)A. The parallelogram denotes a 2D unit cell.



Fig. 2. As-trimer PES for a Ga adatom on In(Al)As(111)A. The parallelogram denotes a 2D unit cell.



Fig. 3. $100 \times 100 \text{ nm}^2 \text{ AFM}$ images of individual (a) 0.6 BL Ge and (b) 4.5 ML GaAs tensile-strained QDs, revealing the difference in their shapes (z-scalebars are 1.5 and 4 nm, respectively). We grew both samples at 535 °C.



Fig. 4. Island scaling analysis performed on (left) Ge and (right) GaAs tensile-strained QDs grown at the same temperature. *S* is the average size of the QDs, θ is the atomic coverage, *i* is the critical cluster size, and *s* is the size of a QD separated into bins. The number of atoms needed to nucleate a quantum dot is *i*+1. After fitting the scaled distributions for the Ge and GaAs QDs we extract critical cluster sizes of *i* = 6 and *i* = 3 respectively, suggesting rather different nucleation behaviors for these two systems.

³ H.S. Lan, S.T. Chan, T.H. Cheng, C.Y. Chen, S.R. Jan, and C.W. Liu, Appl. Phys. Lett. 98, 101106 (2011).

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