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Fine Structures of Ge Nanoclusters on Si(111): STM Observations and First-Principles Theory<sup>1</sup> A.S. RAO, University of Tulsa, H.F. MA, M.C. XU, D.X. SHI, H.J. GAO, Chinese Academy of Sciences, R. GUDIPATI, H.L. DANG, SANWU WANG, University of Tulsa — Germanium-based nanoclusters grown on silicon substrates have potential applications in optoelectronics and nanotechnology. A variety of Ge nanostructures formed on intact Si(111) have been observed. However, the fine structures of the atomic arrangements in the Ge nanoclusters have remained elusive. We performed scanning tunneling microscopy observations and first-principle calculations for investigating the fine structures of the Ge nanoclusters on the Si(111)-7×7 surface. We obtained atomic structures of the nanoclusters formed with a certain process involving deposition at temperature of 423 K and annealing at 550 K. We found that Ge nanocluster, located predominately in the faulted half unit cells of the Si(111)-7×7 surface, contained approximately six Ge atoms with three bonded center Si adatoms. We also observed that the obtained nanostructures were stable up to 600 K.

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