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Investigation on Ge induced GaAs(001)-(1x2) structure JUN NARA, National Institute for Materials Science and IIS, Universityof Tokyo, AKIHIRO OHTAKE, National Institute for Materials Science, TAKAHISA OHNO, National Institute for Materials Science and IIS, Universityof Tokyo — It is known that at the initial stage of the Ge growth on GaAs(001), a reconstructed structure with a (1x2) periodicity is formed. A structure model with Ga-Ge dimers on an As-terminated surface has been proposed for the (1x2) reconstruction. On the other hand, the previous studies have shown that As atoms segregate to the growing Ge surface at the initial growth stages. We have reexamined the atomic structure of the Ge-induced (1x2) reconstruction experimentally and theoretically. We show that the initial growth of Ge on GaAs(001) induces the formation of Ga-As dimers as a result of the site exchange between deposited Ge atoms and subsurface As atoms. We confirmed that this atomic geometry is energetically favored compared with the previously proposed Ga-Ge dimer model, by using first-principles calculations. Our proposed structure model accounts well for the experimental results. This work was partly supported by the RISS project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

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