Stability and mobility of vacancy nanoclusters on Cu(111) surface: An ab initio study\(^1\) ALIREZA AKBARZADEH, ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, California State University Northridge, Department of Physics & Astronomy, 18111 Northridge, CA 91330-8268 — We used ab initio calculations to study stability and mobility of vacancy nanoclusters on Cu(111) surface. We found that the formation energies for single vacancies in the vicinity of the surface are \(\approx 0.3\) eV lower than that in bulk. Interestingly, calculations yield strongly bonded 1st NN divacancy on the surface than in bulk. In addition a trivacancy binds very strong on the surface, indicating that formation of loop-like vacancy nanoclusters are most energetically favored on the surface. These findings imply the ease of nucleation of vacancy nanoclusters on the surface. We also examined migration of mono-, di- and trivacancy on the surface. A zigzag motion for divacancy diffusion on the surface is predicted with the migration barrier higher on the surface than in the bulk due to larger binding energy and elastic contribution.

\(^1\)This research is supported by the National Science Foundations under grant NSF-NIRT CMS-0506841.

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Date submitted: 22 Nov 2008

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