Article

First-Principles Computation of Microscopic Mechanical Properties and Atomic Migration Behavior for Al4Si Aluminum Alloy

Jingtao Huang [1,†], Jingteng Xue [1,†], Mingwei Li [2], Yuan Cheng [3], Zhonghong Lai [4], Jin Hu [1], Fei Zhou [5], Nan Qu [1,*], Yong Liu [1,2,*] and Jingchuan Zhu [1,*]

[1] School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China; 20b909032@stu.hit.edu.cn (J.H.); xuejingteng@stu.hit.edu.cn (J.X.); hujin@hit.edu.cn (J.H.)

[2] National Key Laboratory for Precision Hot Processing of Metals, Harbin Institute of Technology, Harbin 150001, China; limingwei@hit.edu.cn

[3] National Key Laboratory of Science and Technology on Advanced Composites in Special Environments, Harbin Institute of Technology, Harbin 150001, China; cy6810@hit.edu.cn

[4] Center for Analysis, Measurement and Computing, Harbin Institute of Technology, Harbin 150001, China; zhhlai@hit.edu.cn

[5] State Key Laboratory for Environment-Friendly Energy Materials, School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang 621010, China; feizhou@swust.edu.cn

* Correspondence: 18b909065@stu.hit.edu.cn (N.Q.); lyonghit@hit.edu.cn (Y.L.); fgms@hit.edu.cn (J.Z.); Tel.: +86-0451-86413792 (J.Z.)
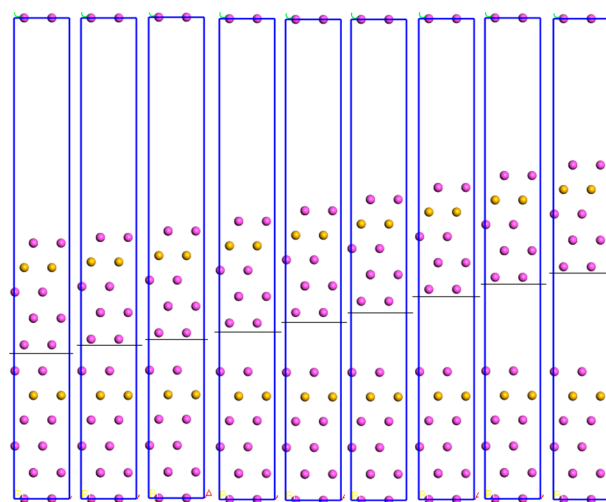
† These authors contributed equally to this work.

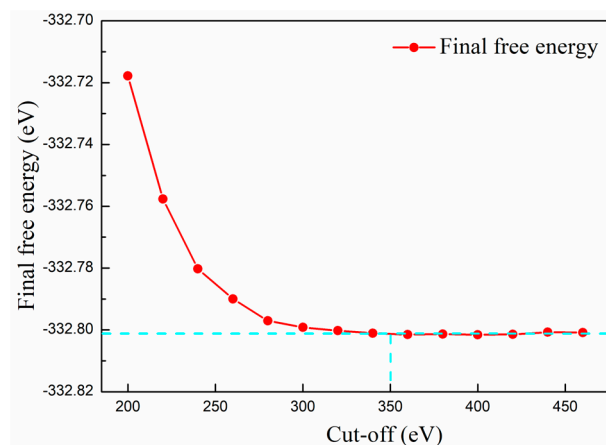**Figure S1.** Schematic diagram of the Al4Si tensile fracture process.

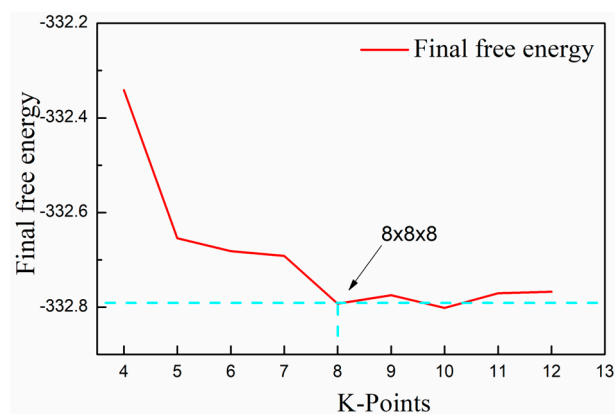**Figure S2.** Cutoff energy convergence test result curve.

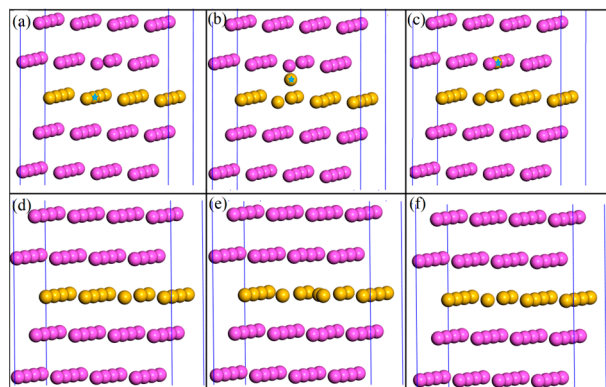**Figure S3.** K-points energy convergence test result curve.

Figure S4. Schematic diagram of diffusive transport pathways.