# Molecular dynamics simulation of complex alloy structures

**Jung Wen Yeh[1], Kouji Tomita[2], Yuuta Imanari[2] and Masaya Uchida[1,3]**

[1]*Department of Information Systems, Graduate School of Engineering, Saitama Institute of Technology, Fukaya, Saitama 369-0293, Japan*

[2]*Department of Information Systems, Faculty of Engineering, Saitama Institute of Technology, Fukaya, Saitama 369-0293, Japan*

[3]*Advanced Science Research Laboratory, Saitama Institute of Technology, Fukaya, Saitama 369-0293, Japan*

*uchida.masaya@sit.ac.jp*

Developing realistic three-dimensional growth models for quasicrystals is a fundamental requirement. Uchida found a general principle for building crystal structures (the *Uchida stacking motif*) in complex alloys such as the μ-$Al_4Mn$ phase [1, 2]. Uchida stacking motif is illustrated in Fig. 1(a)-(c). It comprises three different types of layers—A, B and C—which are stacked in the order C B A B C. The A-layer is a close-packed layer with atomic vacancies. Atoms in the B-layer are located above and below the atomic vacancy sites in the A-layer, while atoms in the C-layer lie above and below interstices in the A-layer. The μ-$Al_4Mn$ phase is a representative approximant crystal, and its structure has a large hexagonal unit cell (with the space group $P6_3/mmc$, lattice constants $a$ = 19.98 and $c$ = 24.673 Å)(Fig. 1(d)). Here, we investigated the Uchida stacking motif using molecular dynamics (MD) simulations to search for clues to the origins of the atomic arrangements in quasicrystals.

We used the LAMMPS code for the MD simulations. Because of the lack of a potential for Mn, all the atoms in the simulation were Al atoms. Thus, we investigated the adsorption of Al on a close-packed Al layer containing one, two or many atomic vacancies as the μ-$Al_4Mn$ phase. The model we used for this close-packed layer was a supercell of Al atoms in an $8a_0 \times 8a_0$ hexagonal cell containing atomic vacancies, where $a_0$ is the Al–Al interatomic distance (Fig. 2(a)). All simulations were performed under the canonical *NVT* ensemble.

The simulation result for the case of the μ-$Al_4Mn$ phase is shown in Fig. 2(b). Our MD simulation results well reproduce the Uchida stacking motif seen in the μ-$Al_4Mn$ phase. The simulations also reveal the formation of a deformed icosahedron. Our results provide new insights into the growth mechanism and origin of complex alloys and quasicrystals.

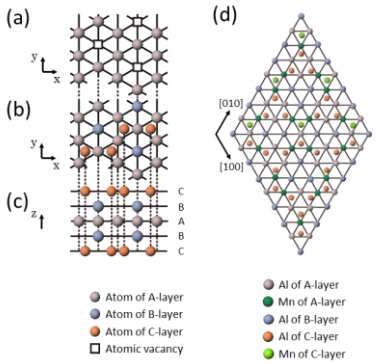


**Figure 1**. The Uchida stacking motif of atoms. (a) Structure in the A-layer. (b) Structures of the A-, B- and C-layers. (c) Side view of the structure. (d) The stacking motif of atoms in the μ-$Al_4Mn$ phase.

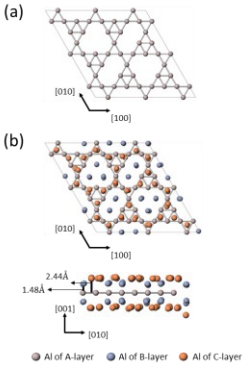


**Figure 2**. (a) Ball-and-stick view of a close-packed layer of Al (the A-layer) with atomic vacancies for MD simulations at 800 K as the μ-$Al_4Mn$ phase. (b) Snapshot of the arrangement of Al atoms adsorbed on the A-layer produced after 1 fs in a MD simulation at 800 K.

[1] Uchida, M. & Matsui. Y. (2000). *Acta Cryst.* B**56**, 654.

[2] Uchida, M. & Horiuchi, S. (1999). *J. Appl. Cryst.* **32**, 417.

**Keywords: complex alloy; quasicrystals; molecular dynamics simulation; stacking motif**