Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A2]Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6

[SY-A2]Combination of Kinetic Monte Carlo Method and First Principles Calculation to Explore Stable Structure of Solute Cluster in Al-Si Based Alloys

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Stable structure of solute cluster in Al-Si based alloys was investigated by combining Kinetic Monte Carlo (KMC) method and first principle calculation. The new KMC code was developed to simulate the behavior of the added impurities in aluminum at finite temperature. The size of KMC cell was $20a_0 \times 20a_0 \times 20a_0$ or $20a_0 \times 20a_0 \times 40a_0$, where a_0 is lattice constant of aluminum. Aluminum atoms were arranged in FCC structure and the impurity atoms of 3at.% or 4at.% was introduced. Diffusion of impurities was performed by swapping two neighbor atoms which was selected randomly. After the swapping, total energy of the KMC cell was calculated and compared with the total energy before the swapping. The stable structure of the impurity cluster was explored with repeating this process. The total energy was calculated by adding up the atom energies which was calculated by dividing the total energy by number of atoms in the cluster. The total energy of the cluster was calculated by the first principle method. Because the atom energy calculated once was recorded in the database, the number of the first principle calculation was reduced. Quantum ESPRESSO was used to carry out the first principle calculation. The pseudopotential file of Becke-Lee-Yang-Parr function was used for Al, Si, Mg, Cu, Zn, Zr, Ti and Ag. The k-point mesh based on Monk horst-Pack (4×4×4) was used to integrate Brillouin zone and the cut off energy of plane wave was 30 Ry. The size of supercell was $2a_0 \times 2a_0 \times 2a_0$, where a_0 is 0.404 nm. The cluster consisted of a central atom and the first neighbor atoms in FCC was arranged in the center of the supercell. The energy of an isolated cluster was calculated. Calculations for binary system (Al-Si, Al-Mg, Al-Cu, Al-Zn, Al-Zr, Al-Ti, Al-Ag), ternary system (Al-Si-Mg, Al-Zn-Mg, Al-Si-Cu, Al-Mg-Cu,Al-Mg-Zr) and quaternary system (Al-Si-Mg-Cu, Al-Si-Mg-Zr, Al-Cu-Mg-Ag) were carried out.