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希ガス照射によるタングステンナノ構造形成理解のための第一原理シミュレーション
First Principles Investigation on Noble Gas Embedded Tungsten

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Introduction

It is reported that tungsten, which is candidate material for the divertor plate in a thermonuclear fusion reactor, is cracked by helium irradiation. The cause of the crack is that irradiated helium creates the bubble structure called 'helium bubble'. Since the crack of tungsten material becomes problem of the use in the reactor, extensive tests of helium irradiation were performed. Moreover, it was experimentally found that helium irradiation generates fuzzy structure in/on tungsten surfaces via helium bubble under the specific conditions of surface temperature, influence and irradiation energy [1]. The fuzzy structure has a potential for functional nano-material beyond the nuclear fusion research field.

Although the condition to generate bubble and fuzzy structures by helium irradiation was made clear experimentally, their formation mechanisms are not clarified. One expectation from experiments is that a key point of bubble structure creation is trap phenomenon of helium atoms into thermal vacancy of tungsten lattice structure. In this context, the binding energies of helium atoms in tungsten material are evaluated by use of first principle calculation based on density functional theory (DFT) [2].

Method

First-principles calculations of the binding energies between noble gas atoms and mono-vacancies of tungsten are performed with the 'OpenMX' code package, which is designed for nano-scale material simulations based on DFT [3].

The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional is used for exchange-correlation potential. Linear combinations of pseudo-atomic localized orbitals, norm-conserving pseudopotentials, and projector expansions are employed for core Coulomb potential. The Brillouin zone with 6x6x6 k-points sampling using the Monkhorst-Pack method is employed.

Iterative calculations of self-consistent field (SCF) convergence and molecular dynamics according to the resulting force are performed to obtain a relaxation state. For the geometry optimization, the Broyden-Fletcher-Goldfarb-Shanno method is employed.

Results

Binding energies and total binding energy of 3x3x3 super-cell consisting of 53 tungsten atoms with mono-vacancy and helium atom(s) are evaluated. It shows that tungsten mono-vacancy can contain at least 9 helium atoms. It is also found that 6 mono-vacancy trapped helium atoms form a kind of cluster structure of octahedral configuration, and the cluster structure is tightly bounded around a mono-vacancy located at center of tungsten cube.

In this presentation, calculated binding energies for the cases of neon and argon will be shown as well.

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