ABSTRAK

Studi ini menentukkan *bravais lattice* yang sesuai dalam pembentukan Cu-Pd alloy berbasis *density functional theory* (DFT). Pembentukan CuPd alloy membutuhkan energi formasi dari *bulk* Cu dan *bulk* Pd. Pada studi ini menghitung energi formasi CuPd alloy secara terpisah-pisah. Sebelum menghitung energi formasi, *bulk* Cu, *bulk* Pd dan CuPd *alloy* dikalkulasikan untuk mendapat keadaan teroptimisasi. Parameter-parameter yang dikalkulasikan adalah *k point*, *cutoff energy* dan *lattice constant*. Hasil kalkulasi pada *bulk* Cu dan *bulk* Pd masing-masing cenderung berbentuk *lattice* fcc dengan energi total sebesar -2899,2668 eV dan -4504,4297 eV berturut-turut. Sedangkan energi total CuPd alloy -7403,9152 eV, -7400,9387 eV, -7402,9556 eV untuk *lattice* sc, bcc, dan fcc berturut-turut. Energi formasi CuPd alloy paling rendah pada *lattice* sc. CuPd alloy cenderung berbentuk *lattice* sc daripada bcc dan fcc.

Kata kunci: *Bulk* Cu, *Bulk* Pd, CuPd *alloy*, *Density Functional Theory*, *Lattice Constant*, dan Energi Formasi.

ABSTRACT

This study determines the appropriate bravais lattice in the formation of CuPd alloy based on density functional theory (DFT). The formation needs formation energy from bulk Cu and bulk Pd. This study calculates the formation energy CuPd alloy separately. Before calculate the formation energy, bulk Cu, bulk Pd and CuPd alloy were calculated to get the optimized state. The parameters that were calculated from them are k-point, cutoff energy and lattice constant. Calculation result on bulk Cu and bulk Pd are tend to be in the form of lattice fcc with total energy -2899.2668 eV and -4504.4297 eV. The total energy of CuPd alloy are -0.2187 eV, 2.7570 eV, and 0.7409 eV for lattice sc, bcc, and fcc respectively. The lowest formation energy of CuPd alloy is in lattice sc. CuPd alloy tend to be in form of lattice sc than bcc and fcc.

Keywords: Bulk Cu, Bulk Pd, CuPd Alloy, Density Functional Theory, Lattice Constant, dan Formation Energy