## AC06

# Spin Reorientation Transition of Ultrathin Body-Centered -Cubic Au/Ni Films

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In thin film magnetism, the materials composed of typical 3d transitional metal elements have been extensively explored. As well known, the Fe, Co, and Ni have body-centered-cubic (BCC), hexagonal-close-packed (HCP), and face-centered-cubic (FCC) crystal structures in bulk mode, respectively. To date, the fundamental magnetic properties of these materials in bulk state are well understood. On the other hand due to the advanced atomic manipulation technique, it is possible to materialize artificial nano structure which does not exist in nature. This brings a new opportunity to utilize the noble magnetic properties for potential magnetic device applications. For instance, Fe and Co used to have BCC and HCP crystal structures in bulk structure can maintain FCC phase under certain conditions [1-3]. This means that the thermodynamically stable crystal structure can be even tuned in an artificial way. Nonetheless, there was no experimental report on the magnetic property of BCC type Ni and it has long been remained an intriguing issue to materialize BCC Ni for experimentalists until recently although the magnetic properties of bulk- type BCC Ni have been studied using first principles method [4-7]. Here, the thickness dependent magnetic properties of artificially prepared ultrathin body-entered cubic Ni films have been explored using the all electron full potential linearized augmented plane wave (FLAPW) method. Two types of BCC Ni(001) film: (i) pure BCC Ni(001) and (ii) Au capped BCC Ni(001) in the range from 1 monolayer (ML) to 5 ML of Au capping coverage have been considered in this report. The magnetic moments of pure BCC Ni(001) has about 0.53 $\mu_B$ in the central layer and a typical surface enhancement is found with magnetic moment of about 0.78 $\mu_B$. In the presence of Au capping layer, the magnetic moment of interface Ni is strongly suppressed to approximately 0.5 $\mu_B$. Nevertheless, the Au adlayer has no meaningful induced magnetic moment. The BCC pure Ni(001) films have always in-plane magnetization up to 11 ML, but very interestingly the Au/Ni(001) shows thickness dependent spin reorientation transition from in-plane to perpendicular to the film surface according to the Au coverage. However, the thickness dependent SRT shows irregular behaviors. In addition, the calculated X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) have been presented. y magnetic circular dichroism (XMCD) have been presented.

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (KRF-2006-331-C00105)

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## AC07

# A First-Principles Study on Magnetic and Electronic Properties of a Ni Impurity in bcc Fe

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Fe-Ni alloys are of interest in connection with Invar effects and martensitic transformations from austenite to martensite at low temperatures. Fe-Ni systems are very important for understanding of steels, especially for their mechanical and magnetic properties.

Very recently we calculated the effects on the magnetic and electronic properties of transition metal impurities in bcc Fe for silicon steels and found that Ni substitution in bcc Fe has the largest averaged Fe magnetic moment among the other transition metal impurities [1]. To understand the magnetic behavior due to the Ni impurity in bcc Fe, we have investigated the magnetic and structural relaxations in terms of first-principles calculations by using the all-electron full-potential linearized augmented plane wave (FLAPW) method [2] as embodied in the QMD-FLAPW package within the generalized gradient approximation (GGA). The calculations are carried out for a 3×3×3 supercell of bcc Fe, which corresponds to 27 atoms in the unit cell and the body centered Fe atom is replaced by Ni. The valence electrons are treated scalar relativistically initially, and then spin-orbit couplings (SOC) are included by the second variation method [3].

The equilibrium lattice constants of the nonmagnetic (NM) state and the ferromagnetic (FM) state are found to be 2.76 Å and 2.84 Å, respectively. The calculated equilibrium lattice constant of the FM state is increased slightly by 0.01 Å compared with the calculated equilibrium lattice constant of pure bcc Fe (2.83 Å). The calculated unit cell averaged Fe magnetic moment, 2.33 μB, is found to be increased upon Ni substitution compared with pure bcc Fe (2.22 $\mu_B$). The analysis on the spin decomposed numbers of charges reveal that the increment of average magnetic moments of Fe sites are mainly due to the spin flips of the Ni impurity atom and its nearest neighboring Fe atom as well as due to small increments of sp electrons of both spins of Ni atom. The amount of the magnetic moments enhancements due to Ni substitution is consistent with the experimental observations [4].

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