Computational and Experimental Evidences for Asymmetric Interfacial Mixing of Co–Al system

Sang-Pil Kim[1,2], Jae-Young Park[3], Kwang-Ryeol Lee[1], Chung-Nam Whang[3], and Yong-Chae Chung[2]

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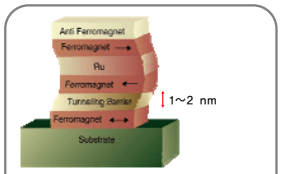
I. ABSTRACT

Asymmetric interfacial mixing behavior of Co–Al system was investigated from computational and experimental approach. Using classical molecular dynamics simulation, when Al atom was deposited on Co surface, atomically sharp interface was formed between the deposited Al layer and Co substrate. On the other hand, when Co atom was deposited on Al(001) surface, atomic intermixing was easily achieved at the interface, and highly ordered CoAl compound phase of B2 structure was formed spontaneously. From experimental approaches by using coaxial impact collision ion scattering spectroscopy (CAICISS) and magneto-optical Kerr effect (MOKE), theses asymmetric intermixing phenomena were confirmed.

II. INTRODUCTION

Scale Down → Major Issue → Solutions



Typical structure of spintronic device

Micro & Bulk Structure Growth & Diffusion

↓

Interfacial Structure Growth & Diffusion **in atomic scale**

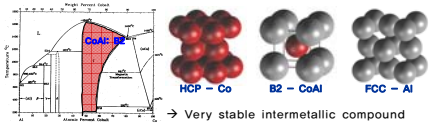
Computational approach + **Experimental approach**

- As the scale of the devices goes down to an atomic level, ***atomic scale control and understanding*** is one of the prerequisite for the success in the development.
- In spintronic devices such as TMR or GMR, the electro-magnetic properties are largely dependent on the interface structure between layers.
- We focused on the asymmetric intermixing behavior of Co–Al system and confirmed by computational and experimental approaches.

III. EXPERIMENTAL DETAILS

Computational Method

- x,y → Periodic Boundary Condition
  z → Open surface (fixing the bottom-most two layers)
- Substrate temperature: 300 K
- Time step: 1 femto-second(fs)
- Deposition rate: 5000fs/atom



→ Very stable intermetallic compound

Co–Al EAM Potentials

Property	Co[1]		CoAl(B2)[2]		Al[3]	
	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.
a_0 (Å)	2.507	**2.512**	2.86	**2.867**	4.05	**4.049**
E_{coh} (eV)	4.39	**4.29**	4.45	**4.468**	3.36	**3.39**
B (GPa)	180	**185**	162	**178**	79	**79.4**

1) R. Pasianot et al., , PRB **45** 12704 (1992). 2) C. Vailhé et al. J. Mater. Res., **12** No. 10 2559 (1997). 3) A. Voter et al, MRS Symp.Proc. , 175 (1987).

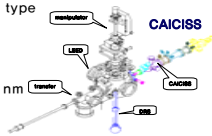
Experimental Method

Sample preparation

- **Metal substrate cleaning:** annealing at 650K for 1–2 hours and sputtering with 2.0 keV Ar^+ ions for several tens of minutes.
- **Deposition process:** evaporation using a heated pure metal (Co, Al) wire.

CoAxial Collision Ion Scattering Spectroscopy (CAICISS)

- **Base pressure:** ~10–11 Torr
- **Probing beam:** 3keV He^+, 3nA(unchopped), 50pA(chopped)
- **Penetration depth:** 〈10 Å
- **Analyzer:** Time-of-flight (TOF) type

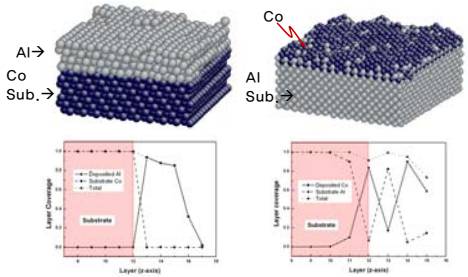


MOKE measurement

- **Wavelength of the light:** 632.8 nm
- Magnetic field was applied **parallel to the sample surface.**
- **Samples:** well controlled electron beam evaporation system for MOKE experiments are Co layer only (reference), Al/Co and Co/Al films.
- Samples are capped by Cu film to prevent oxidation.

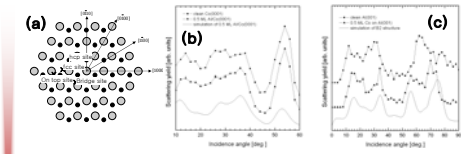
IV. RESULTS and DISCUSSION – 1. Asymmetric Intermixing Behavior

MD Simulation

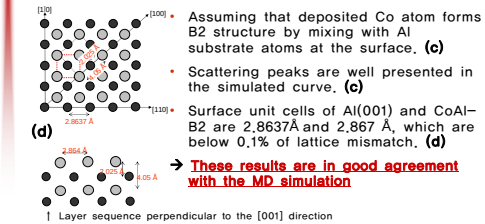


- Layer by layer growth of an Al thin film on Co surface was observed.
- From the layer coverage, it is clearly observed that sharp interface evolved on the surface. (Left figures)
- Most of the deposited Co atoms were mixed with Al substrate and ordered B2–CoAl intermetallic compound was formed. (Right figures)
- Layer coverage shows a zigzag pattern spans up to 3 layers, which indicates formation of B2 structure.

Experiment



- Based on the MD results, assuming that Al atoms were landed on Co(0001) surface. **(a)**
- This results indicate that deposited Al atoms are placed on the hollow site (hcp and fcc site) of Co surface. **(b)**



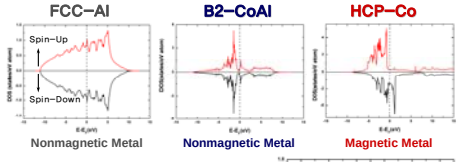
- Assuming that deposited Co atom forms B2 structure by mixing with Al substrate atoms at the surface. **(c)**
- Scattering peaks are well presented in the simulated curve. **(c)**
- Surface unit cells of Al(001) and CoAl–B2 are 2.8637Å and 2.867 Å, which are below 0.1% of lattice mismatch. **(d)**

→ **These results are in good agreement with the MD simulation**

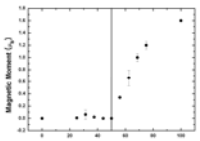
↑ Layer sequence perpendicular to the [001] direction

IV. RESULTS and DISCUSSION – 2. Magnetic Properties

DFT Simulation*

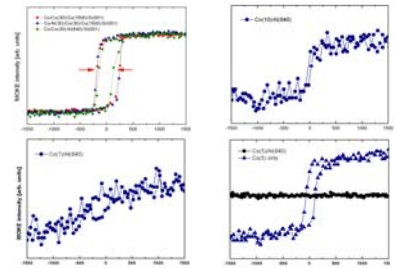


- Al-rich Co_xAl_{1-x} ($x < 0.5$), no apparent ferromagnetism was represented.
- Magnetic moment was rapidly increased with Co concentration in the range above 50 atomic%, and was saturated at a level of pure HCP Co system.
- Co atoms were found to play a critical role in the enhancement of the magnetic moment, and magnetic behavior is also sensitive to surrounding atoms.



* S.-P. Kim *et al.*, IEEE Trans. Magn., 41(10), 3343 (2005).

Experiment



- Shapes and widths of hysteresis loops for Co(30 Å) and Al(30 Å)/Co(30 Å) are almost same.
- Because nonmagnetic B2–CoAl is formed at the interface, width of hysteresis loop for Co(30 Å)/Al(840 Å) sample is narrowed.
- With changing the thickness of Co layer in the Co/Al film, the shape of Co ferromagnetic hysteresis appeared from the case of 5 Å–thick Co film.

V. CONCLUSIONS

- Our results demonstrate the evidences on the asymmetric intermixing behavior of Co–Al system from computational and experimental approaches.
- The combinational techniques of MD, DFT simulations and CAICISS, MOKE experiments can be very powerful and successful tools for the atomic-scale metal on metal system with ML coverage range.

Hanyang University

1. Future Technology Research Division, KIST, Seoul, South Korea 2. Department of Materials Science and Engineering, Hanyang University, Seoul, South Korea
3. Institute of Physics and Applied Physics, Yonsei University, Seoul, South Korea, E-mail: spkim@kist.re.kr (S.-P. Kim), krlee@kist.re.kr (K.-R. Lee)