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Electronic and magnetic properties of interfaces of Ni with Ag/Cu/Au substrates using augmented space formalism

Priyadarshini Parida, Biplab Ganguli *

Department of Physics and Astronomy, National Institute of Technology Rourkela - 769008, India

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ABSTRACT

We model an interface of Ni as an alloy due to interdiffusion of atoms. Alloy composition is taken different at different layers. We observe significant effect of the interdiffusion on electronic and magnetic properties of each layer. These properties also depend on number of layers of Ni deposited on metal substrates. The study is density functional theory (DFT) based first principle calculation using augmented space formalism (ASF) coupled with recursion and tight binding linear muffin tin orbital (TB-LMTO) methods. The formalism is also extended to sharp interface when interdiffusion is negligible.

1. Introduction

The surface and interface properties of transition metal have applications in high-density magnetic recording devices, integrated optical and electronic devices and as sensors [1–4]. Modification of interface due to interdiffusion may therefore alters interface magnetism for any technological applications. When Ni film is deposited on noble metals using electrolytic deposition, the magnetic dead layers are observed [5], which varies with temperature. Such evidences of "magnetically dead layers" have motivated for theoretical studies [6–16]. All these theoretical studies were carried out only for one and two monolayers (MLs) of Ni overlayers on metal substrate. These studies did not consider roughness of interface due to interdiffusion of atoms between film and substrate. Roughness at the interface is always present due to interdiffusion in a real experimental condition. In Ni/Ag and Ni/Cu, the interdiffusion is observed mainly due to difference in their surface energy [7,17,18]. The intermixing of Ni and Cu atoms in Ni-Cu multilayer is discussed using High kinetic-energy photoelectron spectroscopy method [3]. The abrupt interface and the interdiffusion of atoms at Ni-Ag interface is confirmed experimentally using scanning transmission electron microscopy [19] and TEM analysis [20]. The dynamic evolution of Cu atoms into Ni layer is observed using molecular dynamics simulation [21], for 4 MLs of Ni on Cu substrate. In order to minimize the surface energy in immiscible bulk systems, the surface atoms undergo elastic relaxation [22].

We therefore considered more realistic interfaces due to interdiffusion and with more than one monolayer deposition also to emulate actual physical interfaces. Our systems consist of Ni transition metal on (001) surface of Ag, Cu and Au metals. We carried out the layerwise electronic and magnetic properties. We consider one and two MLs of Ni deposition to compare our results with other reported studies [6–16] and to test the accuracy of our method. A molecular dynamics simulations [17] considered interdiffusion of atoms in Ni/Ag in one ML scale. We have also considered 5% and 10% interdiffusion of atoms at the interface for one ML of Ni overlayer and compare these results with that of sharp interface. Intermixing to the directly adjacent layers of the interface is also confirmed by surface X-ray diffraction and molecular dynamics [23] study of Ni/Cu(001) interface. It is also observed that Ni atoms interdiffuse to the second Cu layer in a study by Green's function technique [16]. Therefore, we have also considered the interdiffusion of atoms upto two MLs with different degrees of disorderness on each side of the interface. Though there is no experimental result available for three ML thick Ni film, a previous [24] study using the present methodology on Fe film provided a result which agrees quite well with experimental observation. Therefore we have also taken three layers of Ni with both sharp and rough (5% interdiffusion of atoms) interface.

2. Computational methods

ASF [25,26] has been a suitable alternative theory beyond mean-fields like coherent potential approximation (CPA) to study disordered alloys. ASF can tackle effectively configuration fluctuations along with accurate description of average properties. This is not possible using CPA. A detailed description of the theory may be found in a number papers [25–27] and book [28]. We present here briefly the central concept of the theory.

* Corresponding author.
E-mail address: biplabg@nitrkl.ac.in (B. Ganguli).

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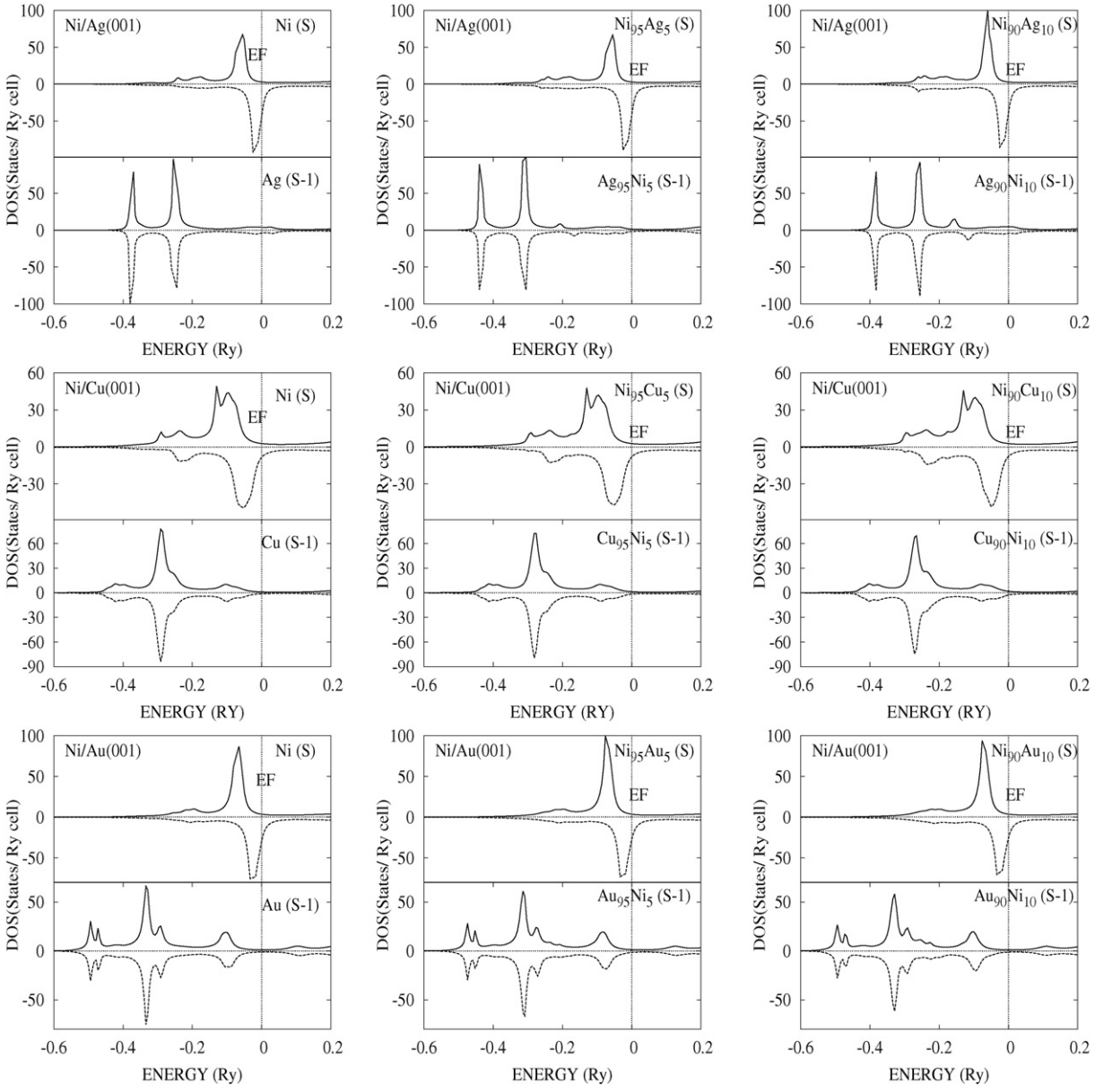

Fig. 1. Layerwise spin polarized DOS for a single layer of Ni deposited on Ag / Cu / Au substrates. S stands for top most layer of the interface. Left panel : $x = 0$ (sharp interface), middle panel: $x = 0.05$ and right panel : $x = 0.1$ (rough interface). Fermi level is reset at zero. Solid line: spin-up and dotted line : spin-down.

The randomness in ASF is described by a set of occupation variables $\{n_i\}$. We assign an operator N_i to each variable $\{n_i\}$. The eigenvalues of N_i are the values taken by n_i and whose spectral density is the probability density of n_i. The ASF Hamiltonian is then constructed by replacing each n_i by its corresponding N_i. In the present case n_i take the values 1 with probability x if site i is occupied by a Ni film layer muffin-tin and 0

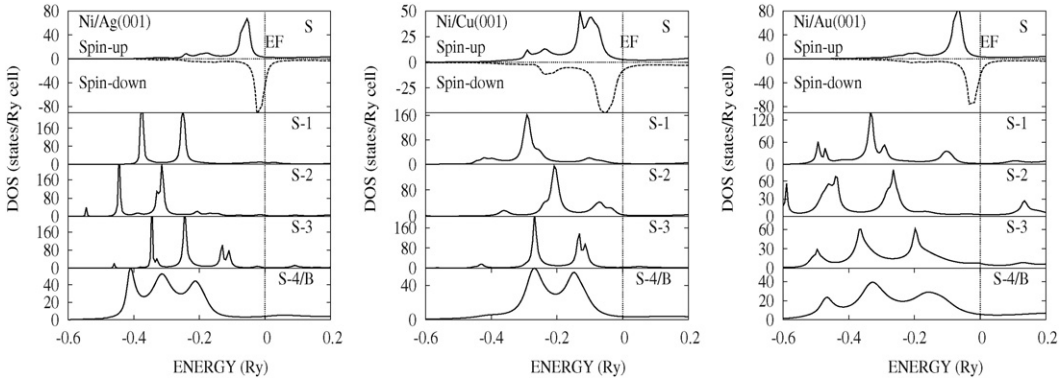

Fig. 2. Layerwise variation of DOS. Fermi level is reset at zero.