

## [III~2]

### The Structure and the Stoichiometry of Ultrathin Films

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#### 1. Introduction

The growth mode and the atomic structure of ultrathin film have affected many physical and chemical properties of the films. Especially magnetic properties of ultrathin film is known to be sensitive to both the growth mode and the atomic structure of the film. The study of the thin film is, however, frequently devastated by the failure in reproducing its properties. These failure is mostly derived from the metastable process involved in the deposition process, because the growth mode is, then, determined by the various local environments affecting the dynamics of the deposited atoms. In real world, the substrate condition is not expected to be perfectly uniform, which implies the growth mode may be more or less different locally. This means that sharply segregated layer by layer growth over the whole surface of the substrate looks improbable. More realistic approach should include the studies of both the atomic structure and the stoichiometry of films. In the current work, we analyzed the LEED I/V characteristics of ultrathin Ni films on Cu(001), Ag(001) and Pt(001) in average t-matrix approximation to find both the structure and the stoichiometry of the films.

#### 2. Average t-matrix Approximation (ATA)

The scattering amplitude for a single scatterer,  $f$ , and t-matrix are defined as

$$\begin{aligned} f(k) &= 2\pi/k \sum_l (2l+1) \sin(\delta_l) \exp(i \delta_l) P_l(\cos\theta) \\ &= 2\pi \sum_l (2l+1) t_l P_l(\cos\theta) \end{aligned}$$

$$t_l = 1/k \sin(\delta_l) \exp(i \delta_l).$$

Diffraction pattern is formed by summing all the scattering amplitude from the crystal lattice. For disordered binary alloys, for example, we cannot simply sum the scattering amplitude. In ATA, the disordered binary alloy (element A and element B) is approximated as a homogeneous crystal formed by *pseudo-atoms* whose scattering property is represented by average t-matrix such as

$$t_{\text{pseudo}} = (t_A + t_B) / 2.$$

The validity of this approximation for binary alloys with large disparity in  $t$ -matrices of alloying elements is well established experimentally[1] and theoretically[2].

### 3. Experiment

Ni ultrathin film was deposited by evaporating Ni from a pure (99.999%) Ni wire in the base pressure of low  $10^{-10}$  torr. The amount of deposited Ni and the cleanliness of the sample was checked by the Auger electron spectroscopy in a conventional way. LEED I/V characteristics was obtained by employing video LEED system.

### 4. Discussion

For the case of Ni/Cu(001) system, due to the similar scattering crosssection of Ni atom and Cu atom, quite a large amount of alloying of Ni and Cu in each layer near the surface does not generate much change in LEED I/V spectra and R-factors. This means that there is large uncertainty in the structure and the stoichiometry predicted by LEED I/V analysis for the systems which show similar scattering properties. Ni/Ag(001) is found to form subsurface disordered alloy, and its kinetic behavior is studied in comparison with Kinetic Tight Binding Izing Model(KTBIM).[3] Ni/Pt system also shows alloying, but still large amount of Ni is left on the surface.

### Reference

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- [3] B. Aufray, H. Giordano, B. Legrand, and G. Treglia, Surf. Sci. **307-309**, 531 (1993).