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Title	Substrate Temperature Dependence of the Atomic Configuration near the Interface in Fe/V Artificial Metallic Superlattice (Commemoration Issue Dedicated to Professor Toshio TAKADA On the Occasion of His Retirement)
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Citation	Bulletin of the Institute for Chemical Research, Kyoto University (1986), 64(4): 181-185
Issue Date	1986-12-06
URL	http://hdl.handle.net/2433/77162
Right	
Туре	Departmental Bulletin Paper
Textversion	publisher

Bull. Inst. Chem. Res., Kyoto Univ., Vol. 64, No. 4, 1986

Substrate Temperature Dependence of the Atomic Configuration near the Interface in Fe/V Artificial Metallic Superlattice

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Received May 16, 1986

The atomic configuration near the interface in the Fe/V superlattice was investigated by ⁵¹V NMR. It was found that the atomic configuration near the interface depends strongly on the temperature of substrate, T_S . From the analysis of the ⁵¹V spin echo spectra, it is suggested that $T_S = -30^{\circ}$ C may be the optimum temperature to minimize the compositional mixing near the interface in the Fe/V superlattice.

KEY WORDS: ⁵¹V NMR/ Fe-V Superlattice/ Interface/ Substrate temperature/

The study of artificial metallic superlattices has received much attention in recent years, since it permits us to expect the appearance of new physical properties in terms of structure, magnetism, superconductivity and so on.¹⁾ In many cases, the compositional mixing occurs necessarily and a topologically two-dimensional alloy region is formed near the interface. The elucidation of the atomic configuration in the interface alloy region is essential so that a technique can be developed to prepare a better quality superlattice which has a structurally coherent and chemically sharp interface. The NMR is an excellent method for the study of local atomic configuration in the interface alloy region, because the observed quantities depend directly on the local electronic states. In Fe/V superlattice, it was reported previously that only one atomic layer at the interface is a concentrated alloy with the Fe(50%)-V(50%) composition and that the compositional mixing is restricted to less than five atomic layers, the latter result having been extracted from the analysis of the ⁵¹V spin-echo spectra.^{2,3)} It has recently been found, however, that the atomic configuration in the interface alloy region depends strongly on the temperature of substrate, T_s . In this paper, we present the results on the T_s -dependence of the atomic configuration near the interface in the Fe/V superlattice.

Three kinds of $Fe(15\text{\AA})/V(30\text{\AA})$ superlattices were prepared by alternative deposition on a mylar substrate under an UHV of 10^{-9} Torr.⁴⁾ The temperature of

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Fig. 1. The ⁵¹V spin-echo spectra at zero external field and 1.3 K, the best calculated distributions of H_n , the estimated chemical composition profiles, and ASRO parameters in the Fe(15Å)/V(30Å) superlattices grown at $T_s = (a) -50^{\circ}$ C, $(b) -30^{\circ}$ C, and $(c) -20^{\circ}$ C. In the upper frame, the curves are the best calculated distributions of H_n , which reproduce the experimental data. The histograms and tales in the lower frame show the estimated Fe concentration x_1^{Fe} and the ASRO parameter α_i in each atomic layer numbered by *i*, respectively.

substrate, T_s , was -50° C, -30° C, and -20° C, respectively. A conventional pulsed NMR spectrometer was used to obtain the ⁵¹V spin-echo spectrum lat zero (or fixed) external filed with changing frequency at 1.3K.

The ⁵¹V spin-echo spectra at zero extenral field in the Fe(15Å)/V(30Å) superlattices are shown by circles in Fig. 1 for three samples: (a) $T_s = -50^{\circ}$ C, (b) $T_s = -30^{\circ}$ C, and (c) $T_s = -20^{\circ}$ C. The signals observed here are associated with the ferromagnetically ordered V sites in the interface alloy region. The spectrum in each sample shows a wide distribution of the internal fields at the V sites, H_{a} , from about -94KOe to -23KOe, and the shape of the spectrum depends strongly on T_s . The negative sign of H_n means the direction of H_n is antiparallel to that of the magnetization of Fe layers. The spectrum associated with the nonmagnetic V interior region is also obtained. The distribution of H_n may be analyzed by using the empirical treatment of the internal field in ferromagnetic alloys, i.e. H_n is assumed to be proportional to the local magnetic moment itself and those of its neighbours. The distribution of the magnetic moments depends on the configuration of Fe and V atoms near the interface in Fe/V superlattice. The atomic configuration in the interface alloy region can be represented by two physical quantities. One is the chemical composition profile, that is the atomic concentration dependence on each atomic layer. The other is the atomic short range order (ASRO). The ASRO parameter a_i in the i-th atomic layer with the concentration of Fe atoms, X_i^{Fe} may be defined as,5)

$$P(X_1^{\text{Fe}}) = X_i^{\text{Fe}} + \alpha_i (1 - X_i^{\text{Fe}}) \tag{1}$$

where $P(X_i^{Fe})$ is the probability of finding an Fe atom at nearest neighbour sites of an Fe atom in the i-th atomic layer. $\alpha_i = 0$ means a random configuration and positive (negative) α_i corresponds to a tendency of clustering (ordering). Then we can estimate the atomic composition and the ASRO parameter in each atomic layer near the interface from the distribution of H_n obtained from the experiment. The details of the analysis were described previously,^{3,6)} and only the result of the analysis is given here.

The estimated chemical composition profile and ASRO parameter in the interface alloy region in each sample are summarized in Fig. 1. The best calculated curves are shown in the same figure, which reproduce the obtained spectra. The result common to all the samples is that only one atomic layer at the interface is a concentrated alloy with the Fe(50%)-V(50%) composition. However, the chemical composition profile and the ASRO parameters vary much from sample to sample; that is, the atomic configuration near the interface depends strongly on T_s . The results of the dependence on T_s are summarized as follows.

- (i) The ASRO parameters in the interface Fe(50%)-V(50\%) layer are positive in the cases of $T_s = -50^{\circ}C$ and $-30^{\circ}C$. On the other hand, it is negative in the case of $T_s = -20^{\circ}C$.
- (ii) The degree of the compositional mixing is small in the case of $T_s = -30^{\circ}$ C (three atomic layers), compared with the cases of $T_s = -50^{\circ}$ C and -20° C (five atomic layers).

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It is a remarkable result that the ASRO parameters in the Fe(50%)-V(50%) layers are estimated to be positive in the samples grown at $T_s = -50^{\circ}$ C and -30° C, which means that the atoms in the interface Fe(50%)-V(50%) layer are likely to cluster among the same kind of atoms. This is very interesting and indicates a clear contrast to the fact that Fe(50%)-V(50%) alloy in the thermal equilibrium has a CsCl-type ordered structure with $\alpha = -1$. We speculate the origin of the positive ASRO parameter in the interface Fe(50%)-V(50%) layer as follows. First, let us consider the situation when the deposition of one species of atom has just been completed. Then, as is shown in Fig. 2, surface atoms are likely to cluster because of the bonding between them. In the following, we imagine the next deposition process on this layer, which is now a substrate surface. If T_s is kept low enough and the kinetic energy of the incoming atoms is small, the atomic configuration of the substrate surface may not be disturbed much when the overlayer is deposited. Thus the ASRO parameter in the interface alloy region may be positive.

Here let us consider the result that the degree of the compositional mixing is smaller in the case of $T_s = -30^{\circ}$ C than $T_s = -50^{\circ}$ C. In the sample grown at $T_s = -50^{\circ}$ C, the interface Fe(50%)-V(50%) layer is situated between Fe(85%)-V(15%) and Fe(15%)-V(85%) layers with a strongly positive ASRO parameter (+0.4). This fact may be interpreted as follows. We suppose again the situation when the deposition of one species of atom has just been completed. If T_s is low enough to suppress the atomic motion on the substrate, the degree of the surface roughness is fairly large as is shown in Fig. 3 (a). When the overlayer is deposited, the rough-



Fig. 2. The schematic illustration of the atomic configuration when the deposition of one species of atom has just been completed.



Fig. 3. The schematic illustration of the atomic configuration when the deposition of one species of atom has just been completed, (a) in the case of lower T_s and (b) in the case of higher T_s .

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ness may remain as it was, so that the degree of the compositional mixing becomes large. If T_s is higher and atomic motion is permitted on the substrate, the surface becomes flatter to gain the binding energy between atoms (see Fig. 3 (b)). Thus the degree of the compositional mixing due to the surface roughness is considered to be smaller as T_s is higher. Therefore, the degree of the compositional mixing may be smaller in the case of $T_s = -30^{\circ}$ C than $T_s = -50^{\circ}$ C.

On the other hand, the ASRO parameter in the interface Fe(50%)-V(50\%) layer was estimated to be negative in the sample grown at $T_s = -20$ °C. This indicates that the interdiffusion between Fe and V atoms develops rapidly with the slight increase of T_s . It is also considered to be due to the effect of the interdiffusion that the degree of the compositional mixing is larger in the case of $T_s = -20$ °C than $T_s = -30$ °C.

Summing up the above discussion about the dependence on T_s , the degree of the compositional mixing due to the surface roughness may decrease as T_s is higher. On the contrary, the degree of the compositional mixing due to the interdiffusion may increase as T_s is higher. Consequently, we speculate from the present analysis of the ⁵¹V spin-echo spectra, that $T_s = -30$ °C may be the optimum temperature to minimize the compositional mixing near the interface in the Fe/V superlattice.

The authors would like to express their sincere thanks to Professors T. Takada, K. Terakura, Y. Fujii, Drs. N. Hamada and N. Hosoito for fruitful discussions.

REFERENCES

- (1) For review, Synthetic Modulated Structures, ed. L. Chang and B.C. Giessen (Academic Press, New York, 1985).
- (2) K. Takanashi, H. Yasuoka, K. Kawaguchi, N. Hosoito and T. Shinjo: J. Phys. Soc. Jpn., 53 4315 (1984).
- (3) N. Hamada, K. Terakura, K. Takanashi and H. Yasuoka: J. Phys. F: Metal Phys., 15 835 (1985).
- (4) N. Hosoito, K. Kawaguchi, T. Shinjo, T. Takada and Y. Endoh: J. Phys. Soc. Jpn., 53 2659 (1984).
- (5) J.M. Cowley: Phys. Rev. 77, 669 (1950).
- (6) K. Takanashi: ScD Thesis, University of Tokyo (1986).