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Review

The influence of radiation-induced vacancy on the formation of thin-film of compound layer during a reactive diffusion process

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ABSTRACT

A theoretical approach is developed that describes the formation of a thin-film of *AB*-compound layer under the influence of radiation-induced vacancy. The *AB*-compound layer is formed as a result of a chemical reaction between the atomic species of *A* and *B* immiscible layers. The two layers are irradiated with a beam of energetic particles and this process leads to several vacant lattice sites creation in both layers due to the displacement of lattice atoms by irradiating particles. *A*- and *B*-atoms diffuse via these lattice sites by means of a vacancy mechanism in considerable amount to reaction interfaces *A*/*AB* and *AB*/*B*. The reaction interfaces increase in thickness as a result of chemical transformation between the diffusing species and surface atoms (near both layers). The compound layer formation occurs in two stages. The first stage begins as an interfacial reaction controlled process, and the second as a diffusion controlled process. The critical thickness and time are determined at a transition point between the two stages. The influence of radiation-induced vacancy on layer thickness, speed of growth, and reaction rate is investigated under irradiation within the framework of the model presented here. The result obtained shows that the layer thickness, speed of growth, and reaction rate increase strongly as the defect generation rate rises in the irradiated layers. It also shows the feasibility of producing a compound layer (especially in near-noble metal silicide considered in this study) at a temperature below their normal formation temperature under the influence of radiation.

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1. Introduction

It is a well-established fact that irradiation creates defects in solid materials [1]. These defects are called radiation-induced defects and the simplest of them is termed a Frenkel pair (vacancy–interstitial pair). By means of radiation-induced defects many new channels are created for atomic diffusion in the target material. Atomic diffusion is very important for layer formation in solid-state reaction. The growth of a compound layer at the reaction interface requires both diffusion and a chemical reaction. This process is termed reactive diffusion.

The phenomenon of reactive diffusion is observed experimentally under both non-irradiation [2–5] and irradiation [6–9] conditions. The compound layer growth is shown to obey parabolic law (thickness is proportional to square root of time) in both cases.

In this paper the influence of radiation-induced vacancy is

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considered on the growth of the compound layer during a reactive diffusion process. Although both vacancy and interstitial defects are created at the same time during irradiation, we take into consideration the situation whereby the contribution of interstitial defect is separated from that of vacancy. With this approach, we are able to determine the contribution of vacancy defects to the growth of a compound layer. We begin by considering the chemical reaction rate as the approximation of product of reactants' atom number densities and assume that the growth rate of the compound layer is proportional to the reaction rate during both interfacial-reaction- and diffusion-controlled stages. Different defect generation rates are taken into account in each irradiated layer in order to determine how it influences the speed of growth, reaction rate, and thickness of a compound layer at a temperature below the compound layer formation under normal heat treatment processes such as conventional furnace and rapid thermal processing.

2. Model and basic equations

Suppose the irradiation of *A*- and *B*-layers leads to the creation of vacancy and interstitial atoms. Let us not consider a very high rate of defect generation; for example, which corresponds to reactor irradiation. In this case, the concentration of interstitial atoms is small, the correlation between fluxes of vacancy and interstitials is weak, and contributions of vacancy and interstitial mechanisms of diffusion can be considered separately. The vacancy mechanism is investigated in the present work.

The number of vacancies in the *AB*-layer increases as the radiation-induced vacancy adds up to the thermally generated ones. We assume that *A*- and *B*-atoms diffuse via a vacancy mechanism through the *AB*-compound layer to reaction interfaces *A/AB* and *AB/B* to form *AB*-compound layer. The thickness of the *AB*-layer formed owing to chemical reaction at interfaces *A/AB* and *AB/B* are designated by $g_a(t)$ and $g_b(t)$ respectively. The total thickness of the compound layer is given by $g(t)=g_a(t)+g_b(t)$. Let the *x*-axis be perpendicular to all the layers under consideration and $g(t)=0$ before irradiation.

The diffusivity of *A*- and *B*-atoms through the vacancy mechanism under irradiation are $D_a^{v,irr}$ and $D_b^{v,irr}$ respectively, and the equation relating the diffusivity under irradiation to that of thermal diffusion is given by:

$$D_a^{v,irr} = \frac{n_a^v D_a^{v,th}}{n_a^{v,th}} \text{ and } D_b^{v,irr} = \frac{n_b^v D_b^{v,th}}{n_b^{v,th}}. \tag{1}$$

where $n_a{}^v$ and $n_b{}^v$ are vacancy concentrations under irradiation, $D_a{}^{v,th}$ and $D_b{}^{v,th}$ are diffusivities of *A*-and *B*-atoms via vacancy mechanism due to thermal vacancies, and $n_a{}^{v,th}$ and $n_b{}^{v,th}$ are thermal vacancy concentrations for *A*- and *B*-atom sites inside the *AB* layer.

Neglecting the recombination between vacancy and interstitial atoms, we can consider the change of densities of vacancy and interstitial atoms separately and obtain equations for two kinds of vacancy concentrations in the *AB* layer:

$$\frac{dn_a^v}{dt} = Kn_a^0 - \frac{\left(n_a^v - n_a^{v,th}\right)}{\tau_a^v} \text{ and } \frac{dn_b^v}{dt} = Kn_b^0 - \frac{\left(n_b^v - n_b^{v,th}\right)}{\tau_b^v}. \tag{2}$$

where K is the defect generation rate, $n_a{}^0$ and $n_b{}^0$ are the number densities of *A*- and *B*-lattice atoms in their respective layers, and $\tau_{v,}{}^a$ and $\tau_v{}^b$ are life-times for *A*- and *B*-vacancy. Because the relaxation of vacancy distribution occurs more quickly than the growth of the *AB*-layer, we assume that the vacancy distribution is homogeneous and stationary: $dn_a{}^v/dt=0$ and $dn_b{}^v/dt=0$.

Thus, for *A*- and *B*-vacancy concentrations we obtain:

$$n_a^v = Kn_a^0\tau_a^v + n_a^{v,th} \text{ and } n_b^v = Kn_b^0\tau_b^v + n_b^{v,th}. \tag{3}$$

Neglecting transient diffusion, we obtain equations for stationary concentration of *A* and *B* atoms inside the *AB* layer:

$$D_a^{v,irr}\frac{\partial^2 n_a(x)}{\partial x^2} = 0 \text{ and } D_b^{v,irr}\frac{\partial^2 n_b(x)}{\partial x^2} = 0 \tag{4}$$

with corresponding boundary conditions:

$$J_a(x=g_b) = R_a = \nu_a\gamma n_b^0 n_a(x=g_b);\quad J_b(x=-g_a) = R_b = \nu_b\gamma n_a^0 n_b(x=-g_a);$$
$$n_a(x=-g_a) = n_a^0;\quad n_b(x=g_b) = n_b^0$$

where J_a and J_b are the fluxes of *A*- and *B*-atoms, R_a and R_b represent the chemical reaction rate at *A/AB* and *AB/B* interfaces and they are not exactly the same, ν_a and ν_b are the stoichiometric coefficients of *A*- and *B*-atoms, and γ is the reaction rate constant. The fluxes of *A*- and *B*-atoms are assumed to occur at the same rate as the chemical reaction in order to ensure that the reaction only occurs at the interface and not inside either the *A*- or *B*-layer bulk.

The speed of growth of the *AB*-layer by virtue of chemical reaction at *A/AB* interface is

$dg_a/dt=V_{ab}R_a=V_{ab}\gamma\ n_a{}^0 n_b\ (x=-g_a)$ and at *AB/B* is $dg_b/dt=V_{ab}R_b=V_{ab}\gamma\ (n_b{}^0)^2$, therefore the total speed is $dg/dt=dg_a/dt+dg_b/dt$, and V_{ab} is the volume of one molecule of the *AB*-layer.

By solving (4) with the given boundary conditions, we obtain an expression for the distribution of the *A*- and *B*-atoms inside the *AB*-compound layer:

$$n_a(x) = -\frac{\gamma\left(n_b^0\right)^2}{D_a^{v,irr}}(x+g_a) + n_a^0 \text{ and } n_b(x,t) = \frac{\gamma n_a^0 n_b^0 \nu_b}{D_b^{v,irr} + \gamma n_a^0 \nu_b g(t)}(x-g_b) + n_b^0. \tag{5}$$

3. The growth of the *AB*-layer

The rate of chemical reaction at interfaces of solid layers depends on the number densities of the *A* and *B* atoms in a complex manner. However, if there exists an excess of *A*- (or *B*-) atoms, then the rate of reaction remain the same with a change of the number density of *A*- (or *B*-) atoms [10]. On the other hand, if number densities of the *A*- and *B*-atoms approximately equal $\nu_a n_a \approx \nu_b n_b{}^0$, then the rate of the *AB*-compound formation can be represented in the first approximation as a product of *A*- and *B*-atom number densities.

Thus the rate of chemical reaction between the *A*- and *B*-atoms, at reaction interfaces *A/AB* and *AB/B*, can be approximately expressed in two stages in the following ways:

$$R_a = \begin{cases} \gamma\left(n_a^0\right)^2 = \text{const} & \nu_b n_b(x=-g_a) \geq \nu_a n_a^0 \\ \gamma n_a^0 n_b(x=-g_a) & \nu_b n_b(x=-g_a) \leq \nu_a n_a^0 \end{cases}$$

$$R_b = \begin{cases} \gamma\left(n_b^0\right)^2 = \text{const} & \nu_a n_a(x=g_b) \geq \nu_b n_b^0 \\ \gamma n_b^0 n_a(x=g_b) & \nu_a n_a(x=g_b) \leq \nu_b n_b^0 \end{cases}. \tag{6}$$

Where $n_b\ (x=-g_a)$ and $n_a\ (x=-g_b)$ are number densities of the *B*-atoms at $x=-g_a$ and the *A*-atoms at $x=-g_b$.

Owing to this, approximating the growth of the *AB* layer can have two stages. The first stage is when there is an excess of one kind of diffusing atom; for example, an excess of the *A*-atoms near interface *AB/B* or an excess of the *B*-atoms near interface *A/AB*. The second stage is when there is no excess of any kind of atoms near the corresponding surface; the second stage can take place

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