



*Faculty of Science
Physics Department*

Investigation of Solid State Reaction in Silver/Tin Nanostructured Thin Films

A Thesis

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ABSTRACT

Name : Nora Samy Sdky Mohareb
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The present thesis is devoted to investigate the solid-state reaction in the nanocrystalline Ag/Sn thin film system at room temperature (at about 298K). The investigation includes:

1. The different individual film thicknesses of Ag/Sn system were prepared by Direct Current (DC) magnetron sputtering instrument.
2. The sputtering rates were calculated from the layer thickness measured by profilometer technique.
3. The structure identification of the samples was investigated by X-ray diffraction (XRD) patterns.
4. The elemental composition of the studied samples was measured by Secondary Neutral Mass Spectrometry (SNMS).
5. The Analysis of the SNMS profiles including:
 - Studying the kinetics of the mechanisms based on the grain boundary diffusion process.
 - The velocity of the interface by Diffusion-induced grain boundary motion (DIGM) mechanism was calculated.
 - The growth rate of the Ag₃Sn intermetallic phase by Diffusion-induced recrystallization (DIR) mechanism was estimated.

Keywords: GB diffusion; Thin film reactions; Nanostructure.

CHAPTER 1

THEORETICAL BACKGROUND and

LITERATURE RECIEW

A. THEORETICAL BACKGROUND

Solid-state reactions in nanostructured thin film systems are interesting not only for technological applications, but are important of pure fundamental research [9]. One of the effective bonding techniques is diffusion soldering based on the interdiffusion process in thin films bilayer and multilayer systems of high-melting and low-melting materials [8]. Transport of material by migration of atoms or molecular entities between two layers, i.e. diffusion (Fig. (1.1a)), is one of the most fundamental, elementary processes in materials and, thus, of great importance to the materials scientist and engineer [32]. Diffusion of atoms in solids can be described by Fick's equations.

1.1. Fick's Equations

The first equation relates the flux ($\vec{J}$: number of atoms crossing a unit area per unit time) to the gradient of concentration (ρ : number of atoms per unit volume) via the diffusion coefficient tensor $\hat{D}$:

$$\vec{J} = -\hat{D}\text{grad } \rho \quad (1.1)$$

In general, the diffusion flux and concentration are function of time and position. In order to be able to determine the diffusion coefficient, it is necessary to take into account the conservation of matter. For not interacting particles, this is the continuity equation:

$$\frac{\partial \rho}{\partial t} + \text{div} \vec{j} = 0 \quad (1.2)$$

Combining equations (1.1) and (1.2), one obtains the second Fick's law (or the diffusion equation):

$$\frac{\partial \rho}{\partial t} = \text{div}(\hat{D} \text{grad } \rho) \quad (1.3)$$

For cubic crystals and isotropic media, the diffusion coefficient tensor reduces to scalar D and if the concentration varies only in the x -direction thus, the first Fick's law is:

$$J_x = -D \frac{\partial \rho}{\partial x} \quad (1.4)$$

and second Fick's law reduces to:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial \rho}{\partial x} \right) \quad (1.5)$$

If, additionally, the diffusion coefficient is independent of the concentration, Eq. (1.5) can be written in the following form:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \quad (1.6)$$

From mathematical point of view, Eq. (1.6) is a second order, linear partial differential equation. Initial and boundary conditions are necessary to solve it [33]. Fig. (1.1b) depicts the solution of Fick's second law at different times.

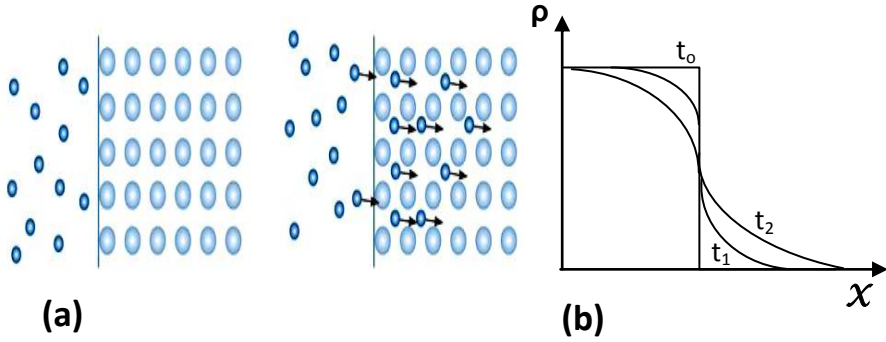


Fig. (1.1): (a) The migration of atoms or molecules, (b) Illustration of the solutions of Fick's second law at different times.

Temperature has a profound influence on the coefficients and diffusion rates. The temperature dependence of the diffusion coefficients is:

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right) \quad (1.7)$$

where D_0 is a temperature-independent pre-exponential (m^2/s), Q_d is the activation energy for diffusion (J/mol), R is the gas constant (8.31 J/mol.K), and T is the absolute temperature [34].

1.2. Expressions for atomic fluxes from first principles and atomistic interpretation

1.2.1 Expression for Atomic Fluxes

According to the second law of thermodynamics, fluxes of extensive quantities are proportional to the gradients of intensive quantities, therefore Fick's first law in A/B binary alloys can be written as: (if the gradients of other intensives than the chemical potential of A atoms are zero)

$$J_A = -L_D \nabla \mu_A \quad (1.8)$$

where L_D is Onsager coefficient, J_A is the atomic flux and μ_A is the chemical potential which has a concentration dependence [35]:

$$\mu_A(c) = \mu_0 + kT \ln \gamma c \quad (1.9)$$

where μ_0 is equilibrium chemical potential of A, k is Boltzmann constant, T is the absolute temperature, γ is the chemical activity coefficient and c is the atomic fraction ($c = N_A/N$), N_A is number of A atoms and N is the total number of atoms. Considering diffusion only along x direction, derivative of μ_A can be expressed as:

$$\frac{\partial \mu_A}{\partial x} = \frac{kT}{c} \frac{\partial c}{\partial x} \left(1 + \frac{\partial \ln \gamma}{\partial \ln c} \right) \quad (1.10)$$

The (1.10) equation – using also Eq. (1.8) and Eq. (1.9) can be divided into two parts. The first, conductive term describes the mixing without external driving force, while the second one corresponds to the driving force comprising from chemical interactions (γ is unity for ideal systems):

$$J_A = -\frac{D_B}{\Omega} \frac{\partial c}{\partial x} - \frac{D_B}{\Omega} \frac{\partial \ln \gamma}{\partial \ln c} \frac{\partial c}{\partial x} \quad (1.11)$$

where $D_B = L_D kT / c$ is the Brownian random walk diffusion coefficient, $D_i = D_B (1 + \frac{\partial \ln \gamma}{\partial \ln c})$ the intrinsic diffusion coefficient and Ω is the atomic volume. The convective term corresponds to a drift velocity v_d and thus: