Kinetic modeling of nanocomposites formation during co-deposition of binary films

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Abstract
The processes occurring during a thin film growth of two immiscible components are investigated by using proposed mathematical models [1, 2]. The proposed model is based on rate equations and includes the processes of adsorption, phase separation, surface segregation, surface and bulk diffusion. The mathematical descriptions of the processes of phase separation and surface segregation are based on the Cahn Hilliard equation and Gibbsian segregation model, respectively. The numerical calculations revealed that the growth rate, diffusion coefficient near the surface D_0, the concentrations of thin film constituents, the solubilities of thin film components were the important factors determining the phase structure of the thin films. Moreover, the numerical results showed that the phase structure was related to the ratio of diffusion coefficient near the surface over the growth rate D_0/V_{ad}. The binary thin films tended to grow in a columnar manner when either the relatively high values of D_0/V_{ad} or the relatively low differences between the contents of both film constituents were used. The surface diffusion dominated during the growth of the columnar structures. The change from a columnar pattern to one containing globular nanoparticles could be achieved either by decreasing the value of D_0/V_{ad}, or by increasing the difference between the contents of the film components. The bulk diffusion was responsible for the formation of globular nanoparticles embedded in another phase. Same transition from a columnar pattern to one containing globular nanoparticles resulted from the increase in solubilities of both components. The influence of the surface segregation on the phase structure during a thin film growth was also analyzed. These modeling results were compared to the experimental data taken from literature where the C:Ni thin films were grown at different contents of Ni and substrate temperatures. The conclusions about the growth mechanisms of the thin films were drawn. This project has received funding from European Regional Development Fund (project No 01.2.2-LMT-K-718-01-0071) under grant agreement with the Research Council of Lithuania (LMTLT) .

References

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[2] G. Kairaitis, A. Grigaliūnas, A. Baginskas, A. Galdikas, Kinetic modeling of phase separation and surface segregation in growing a-C:Ni thin films, Surface Coatings and Technology, 352 (2018) 120–127.

Figures

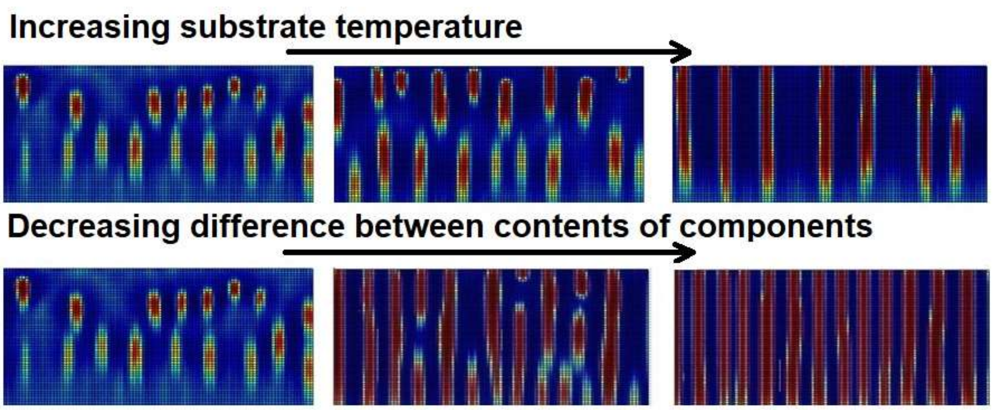

Figure 1. Influence of substrate temperature and thin film composition on phase structure