Phase-Field modeling of the spinodal decomposition in $Zn_{1-x}Cd_xO$ films

I. Shtepliuk [1], **N. Podolskaia**[2,3], **G. Lashkarev**[1]

[1] *Institute for Problems of Materials Science, NASU, 03680, Kiev, Ukraine*
[2] *Ioffe Physico-Technical Institute, RAS, Saint-Petersburg, Russia*
[3] *Saint-Petersburg Branch of Joint Supercomputer Center, Saint-Petersburg, Russia*

$Zn_{1-x}Cd_xO$ alloys are promising candidates for use in optoelectronic applications including visible emitters [1]. It is well known that the designing the high-performance light-emitting devices demands the use of high-quality epitaxial films with no phase separation. Previous investigations showed surprisingly that the $Zn_{1-x}Cd_xO$ thin films demonstrate chemical fluctuations causing the appearance of nanoscale cadmium-rich clusters [2]. This may be induced by a wide miscibility gap of the $Zn_{1-x}Cd_xO$ alloys [3]. For this reason the clear understanding the kinetics of the phase separation in $Zn_{1-x}Cd_xO$ films is very important task.

Here we carried out the analysis of the spinodal decomposition in the $Zn_{1-x}Cd_xO$ ternary alloy by means of the nonlinear Cahn-Hilliard equation. The morphological patterns for the ternary alloys with different Cd content (x=30, 40, 50 %) were obtained using the semi-implicit Fourier-spectral method. An effect of the phase-field mobility and the gradient energy on the microstructure evolution of the $Zn_{1-x}Cd_xO$ alloys is discussed. It was found that the higher driving force for the decomposition in the higher Cd content film results in a higher decomposition rate revealed by the simulations. Moreover, thermodynamic and structural properties of wurtzitic $Zn_{1-x}Cd_xO$ alloy were studied by Valence Force Field method.

Figure 1 shows the microstructural evolution predicted for the $Zn_{1-x}Cd_xO$ alloys with cadmium content of 30, 40 and 50 %. The microstructure was determined using the two-dimension concentration results. As it can be clearly seen from Fig. 1 the microstructure of the $Zn_{1-x}Cd_xO$ ternary alloy is changed with increasing the cadmium content from structure with separate domains (Fig.1a) to interconnected domains (Fig. 1c). The size of decomposed phases in the case of the lowest cadmium content is much smaller than that of highest cadmium content. The interconnected microstructure is more clearly observed in the case of the alloy with 50 at.% Cd than at that corresponding to the other alloy composition. This type of morphology is proper to early stages of the spinodal decomposition. This fact can be attributed to the higher driving force for the phase decomposition in the $Zn_{1-x}Cd_xO$ alloy with x=0.5.

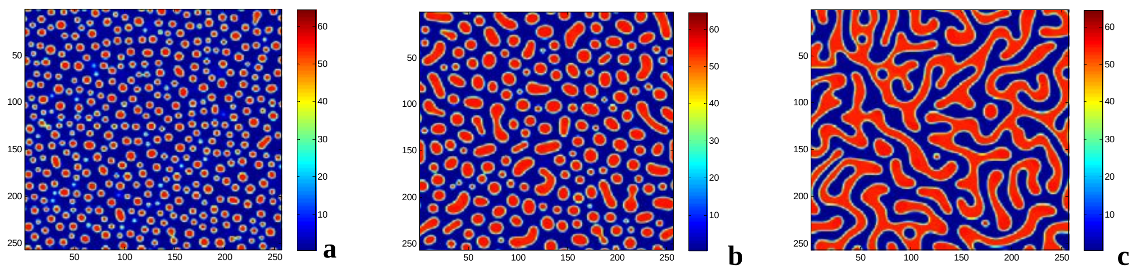

Figure 1 Morphological patterns during spinodal decomposition and subsequent coarsening: a – 30 % Cd, b – 40% Cd and c – 50% Cd. Red color represents the Cd-rich phase and blue is referred to Cd-poor phase.

[1] I. Shtepliuk, V. Khranovskyy, G. Lashkarev et al., *Solid State Electron.* **81**, 72 (2013).
[2] A. Singh, D. Kumar, P. K. Khanna et al., *ECS J. Solid State Sci. Technol.* **2**, Q136 (2013).
[3] I.I. Shtepliuk, *Acta Phys. Pol. A* **124**, 865 (2013).