Application of phase separation model for phase changing of α - to β -metal hydride phase during hydrogen absorption

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Metal hydrides are promising materials to store hydrogen in a solid state. Hydrogen is absorbed into interstitial sites in metal phase and metal hydride phase (α -phase) is evolved as the amount of absorbed hydrogen increases. At certain limit, another metal hydride phases known as β -phase is formed and coexistence of α - and β -phase takes place under isobaric condition. In the present study, the generation and the growth of β -phase was modeled using a phase separation model. The phase change is known as a diffusion controlled phenomenon similar with spinodal decomposition. Therefore, a diffusion equation was set up based on a phase-field theory. Some experimental data were correlated to verify the model. The proposed model would be applied to simulate the absorption behavior of metal hydrides.