

Abstract

Instability to phase separation and nanoscale electronic inhomogeneity are theoretically studied on the basis of microscopic models by using large-scale real-space numerical simulations. The purpose of the study is to fill the missing link between microscopic calculations, which have been performed in small size systems and mainly in one dimension, and phenomenological theories based on many hypotheses in integrating out the microscopic degrees of freedom. The understanding the physics of the electronic inhomogeneity is a key to shed light on the mechanism of many intriguing behaviors in strongly correlated systems such as the colossal magnetoresistance and the colossal electroresistance. Our model is an extended Falicov-Kimball model including the effect of surface and local impurity potentials. The model exhibits an instability toward phase separation in the bulk clean limit. We clarify how the system behaves in the phase separated region in the presence of surfaces and impurities. By employing Monte Carlo method with an advanced technique to reduce the cpu time, we study the real-space structure of domains systematically by changing the electronic correlation, the density of electrons, the structure of surfaces, the strength and the concentration of impurities. The results are also compared to the mean-field results to elucidate the fluctuation effects. As a result, we found that large phase separated domains in the clean limit are broken into small pieces, and that the domain sizes systematically depend on the distance from the surfaces. The results are compared to a phenomenological theory for the colossal electroresistance.