ACTA PHYSICA DEBRECENIENSIS XLI, 99 (2007)

NANODIFFUSION

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According to Fick I law the diffusion kinetics goes to infinity if the diffusion time goes to 0, because the initial gradient can go to infinity. We showed that for the resolution of this longstanding diffusion paradox. One has to take into account not only the atomic scale discrete character (always finite initial gradient) but the finite diffusion permeability of the initial interface (determined by finite atomic jump frequencies across the interface). We found that in a diffusion pair with strong diffusion asymmetry (strongly composition dependent diffusion coefficient), this leads to linear diffusion kinetics and the characteristic crossover thickness between the linear and parabolic kinetics can be estimated. We obtained that it can be even few hundred nm. We presented an atomistic interpretation for the interface mass transfer coefficient, K, determining the linear kinetics. The results are very important for all nanoscale reactions, where non-parabolic behaviour is observed

The Nernst-Planck equation states that the flux is proportional to the driving force. We showed how this equation can be generalized for large diffusion driving forces, if the diffusion asymmetry is strong. We also obtained that for large stress gradients the crossover thickness can be increased by several times.

We showed that changing the substrate thickness, a segregation induced interface diffuseness can indeed be produced: in Mo/V multilayer system the thickness of the V/Mo interface (produced by depositing V on Mo) was independent of the substrate temperature, while the Mo/V interface (produced by deposition of Mo on V) became sharper with increasing substrate

temperature. This was interpreted by the V segregation induced atomic jumps (which compensate the ballistic intermixing). The measurements were carried out on epitaxial Mo/V multilayers, produced by magnetron sputtering, applying in situ heat treatments.

We showed that during the dissolution of thin films into a matrix, the usually assumed local surface equilibrium can be violated, and the calculated surface segregation isotherms can include errors due to deviations from the Fick I law.

This research was supported by OTKA grant K61253.