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Molecular Simulation of Pressure Solution Interfaces – Diffusion and Dynamic Interface Structure

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Pressure solution creep has for a long time been considered as an important ductile rock deformation mechanism in diagenesis of sedimentary rocks. Aggregates of mineral grains in sedimentary basins experience an increasing overburden pressure relative to the fluid pressure as they are buried ever deeper. It is well established that the high stress at grain contacts cause dissolution of the minerals at the grain boundary, transport of the dissolved matter in a fluid phase out of the grain boundary and precipitation of this material in the pore space on the less stressed faces of the grains. There is still considerable debate about the dissolution and transport mechanisms on the microscopic grain boundary scale, notably about the nature of the dissolving solid interfaces and of the confined water.

Computer simulation has already proven to be a good tool for the study of confined fluids. Many studies of confined films under pressure suggest that they are in a solid-like structure. Since most studies have been directed at understanding the solvatation force and rheological behaviour of fluid films in idealized geometries, studies of diffusion mechanisms in such films are lacking but necessary to understand the fundamentals of pressure solution.

We develop a methodology for grand canonical Monte Carlo preparation of the initial configurations for molecular dynamics simulations of confined fluids at geological conditions. We define projections of the density-density time correlation function in a confined geometry and their connections to the static fluid structure and diffusion. We measure these quantities at different thermodynamic conditions corresponding to different burial depths. A solid surface undergoing pressure solution must have a minimal structure of atomic dimensions. We study the effect of atomic scale surface irregularities on breaking the crystalline-like film structure locally and show that atomic scale roughness breaks up the confined fluid structure and enhances diffusion. Based on these results we discuss dissolution smoothening or roughening during pressure solution by diffusion feedback as opposed to plasticity control and we relate this to recent observations by in situ X-ray reflectivity by Wogelius et al. (2000).

Wogelius RA, Dysthe DK, Tang CC, Nield AA, *Goldschmidt 2000 Abstract volume*, (2000).