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Fast Ionic Transport along Interfaces in Minerals

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Mobilities of ions are significantly enhanced when transport occurs along interfaces such as twin boundaries or rims of radiation damaged clusters. A typical example for the latter mechanism is the transport of hydrous species along the rimes between radiation amorphised and crystalline tintanite. IR spectroscopic studies have shown that dehydration of radiation damaged titanite occurs at the percolation point of the interfacial connectivity and not at the percolation point of the amorphised regions themselves. Enhanced transport along twin boundaries was shown experimentally and by computer simulation in minerals with perovskite-type structures such as WO3, PbTiO3 etc. The enhancement is closely related to the ability of such structures to relax atomistically around the transported ion. Interfaces play the role of the ‘elastically soft’ parts of the crystal structure which also leads to the expectation that partition functions are significantly modified by such microstructures. Examples for experimental observations and theoretical models will be presented.