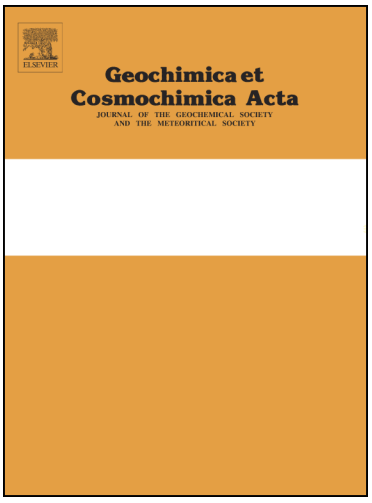

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Dissolution of minerals with rough surfaces

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Abstract

We study dissolution of minerals with initial rough surfaces using kinetic Monte Carlo simulations and a scaling approach. We consider a simple cubic lattice structure, a thermally activated rate of detachment of a molecule (site), and rough surface configurations produced by fractional Brownian motion algorithm. First we revisit the problem of dissolution of initial flat surfaces, in which the dissolution rate r_F reaches an approximately constant value at short times and is controlled by detachment of step edge sites. For initial rough surfaces, the dissolution rate r at short times is much larger than r_F; after dissolution of some hundreds of molecular layers, r decreases by some orders of magnitude across several time decades. Meanwhile, the surface evolves through configurations of decreasing energy, beginning with dissolution of isolated sites, then formation of terraces with disordered boundaries, their growth, and final smoothing. A crossover time to a smooth configuration is defined when $r = 1.5r_F$; the surface retreat at the crossover is approximately 3 times the initial roughness and is temperature-independent, while the crossover time is proportional to the initial roughness and is controlled by step-edge site detachment. The initial dissolution process is described by the so-called