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Modeling the Transport of $K^+$ at Solid-solution Interface by Chemical Potential Gradient and Its Application

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Dissolution of solid material from solutions has widespread applications in advanced material synthesis, oceanography, metallurgy, ceramics, desalination technology, sustained drug release processes, etc. Usually many complex factors affect the dissolution rate in the applications and it is very important to predict and find controllable parameters to control the rate by modeling, which expects a decline in the need for extensive experimental measurements. For example, in the ion exchange process of $K_2Ti_4O_9$ whiskers to produce a kind of advanced material $K_2Ti_6O_{13}$, many factors such as ion exchange time, amount of $H_2O$, concentration of $K^+$, pH value, temperature, etc. influence the process and the ion exchange rate is usually very low, which brings great difficulties for the scaling up of the process for preparing the products with high quality.

When crystals dissolve in solutions, a surface reaction layer and diffusion layer will form in a few microns away from the crystal surface. The chemical potential gradient between the crystal and the solid-solution interface is the driving force of surface reaction and the chemical potential gradient between the solid-solution interface and the bulk phase is the driving force of the diffusion. So it is the most important to investigate the transport at the solid-solution interface for the dissolution process.

In this context, potassium inorganic compounds are selected as model systems. In order to predict the dissolution rate, linear nonequilibrium thermodynamics is applied to describe the transport rate of the surface reaction and diffusion in the dissolution process [1-2]. Statistical rate theory is modified with the correction of the non-ideality of electrolyte solutions to describe the transport behaviors of solid-solution interface more accurately [1-2]. Experimental apparatus with ion selective electrodes is established in which potential-meter is used to detect the cell potential online with 1-second interval [3-4], then the concentrations of $K^+$ at different time is calculated according to the Nernst Equation with the correction of the non-ideality [1-2]. The dissolution rate could be predicted and the resistances of surface reaction and diffusion could be analyzed based on the chemical potential gradient modeling and experimental results. In this presentation, the effects of temperature, stirring speed and solvents on $K_2SO_4$ dissolution are analyzed [1-2]. Moreover, two application cases for carnallite dissolution and ion exchange process of $K_2Ti_4O_9$ with modeling the transport of $K^+$ at the solid-solution interface will be introduced in details [5-7]. And the description of drug dissolution by chemical potential gradient modeling will be summarized.

References:


**Keywords:** Chemical potential gradient modeling, dissolution, linear nonequilibrium thermodynamics, solid-solution interface, potassium ion selective electrode, ion exchange process