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On the Mechanism of Sodic Removal from Bauxite Residue and Bauxite Desilication Products (BDP) Using Microbiogenic Acids

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Bauxite desilication products (BDP) are fundamental causes of persistent alkalinity and salinity in bauxite residue (BR). Previous studies have shown that significant amounts of microbiogenic acids (e.g., CH_3COOH, $H_2C_2O_4$) and Na^+ were detected in the pore water of organic matter-amended and bacteria-colonised bauxite residue, implying the capability of microbiogenic acids to alleviate the alkalinity and salinity of bauxite residue [1]. The present study aims to establish a fundamental understanding of bauxite residue/BDP weathering mechanism by using microbiogenic acids as case models of microbial-derived low-molecular-weight soluble organic compounds. The sodium concentration in microbiogenic acids-treated bauxite residues has significantly decreased in the mineral phase, which is dominated by Na^+-H^+ exchange process with partial breakdown of aluminosilicate β-cages. According to the results from Attenuated total reflection and fourier-transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, and X-Ray photoelectron spectra, it was indicated that acetate and oxalate were adsorbed/complexed on the surface of BDP, causing slight deformation of BDP's cages and thus enhancing surficially encaged Na^+ easily detached from alkaline mineral surface [1-3]. The atomistic molecular dynamic simulation confirmed the adsorption of the microbiogenic acid molecules on the cleaved (110) surface of hydroxylsodalite, through either interactions with Al or Si atoms of the β-cages or hydrogen bonding with surface oxygen atoms. In addition to critical Na^+- H^+ exchange process, the adsorption of microbiogenic acids on BDP also contribute to triggering surfacial Na^+ diffusion into aqueous solution from hydroxylsodalite *b*-cages. These collectively suggested that the continuous Na^+- $H^+_{(organic)}$ exchange process mediated by the organic acid complexation would be critical to the depletion of BDP and dealkalization of the treated bauxite residue in the long-term, preventing future release of Na into the soluble phase and the reversal of the alkalinity. These findings may lead to unlocking the barriers to sustainable bauxite residue rehabilitation.

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[2] Wang, S., et al. (2020) *JOM 72*, 309-318.

[3] Huang, L. et al. (2018) *Alumina Conference*, Australia.