Recepción de resumenes CCG

Titulo / Autores / Institución

TITULO DE LA PONENCIA

Exploring Boron Isotope Fractionation: The Role of Melt Structure and Cationic Effects in Silicate Systems

AUTORES

Paola Patron, Carlos Pinilla y Sadro Jhan

INSTITUCIÓN

Universidad del Norte

CORREO ELECTRÓNICO

patronp@uninoredu.co

Estilo preferido

ESTILO DE PRESENTACIÓN

- Poster

Categoría del resumen

ÁREA TEMÁTICA

Inteligencia Artificial

LINEAS TEMÁTICAS AI

Inteligencia Artificial

Resumen

PALABRAS CLAVE

machine learning, isotope fractionation, borosilicate melts

CONTENIDO DEL RESUMEN

Boron is a moderately volatile, fluid-mobile, and lithophile element with two stable isotopes, ^{10}B and ^{11}B, occurring at a 4:1 ratio and exhibiting a ~10% relative mass difference, making it highly susceptible to isotope fractionation. Geologically, boron is mobile in magmatic systems and often enriched through sediment assimilation and fluid interactions. In silicate melts, boron exists as BO_3 and BO_4 units, interacting with network-forming elements such as Si and O to form complex structures, including tourmaline (Archer et al., 2003; Paz and Langel, 2020). However, while isotope fractionation is well characterized in surface fluids, data from deep mantle regions remain limited and unclear (Kowalski et al., 2013; Dawson and Roberts, 2022; Jahn, 2022;). Due

to analytical and sampling limitations in high-temperature experiments, theoretical and computational methods offer a valuable approach to understanding boron behavior in melts (Wang and Zhang, 2017; Zhu and Li, 2020). This study employs molecular dynamics simulations enhanced by machine learning-derived interatomic potentials, trained on DFT data, to investigate boron isotope fractionation in sodium-rich borosilicate melts under high-temperature conditions, analyzed structural properties, BO_3/BO_4 coordination, and configurational effects. This study employs molecular dynamics simulations enhanced by machine learning-derived interatomic potentials, trained on density functional theory (DFT) data, to model boron isotope fractionation in sodium-rich borosilicate melts under high-temperature conditions. We analyze structural properties, BO_3/BO_4 coordination, and configurational effects, providing a novel and cost-effective approach to studying isotope behavior in extreme environments

REFERENCIAS BIBLIOGRÁFICAS

Archer, T. D., Birse, S. E. A., Dove, M. T., Redfern, S. A. T., Gale, J. D., and Cygan, R. T. (2003). An interatomic potential model for carbonates allowing for polarization. Geochimica et Cosmochimica Acta, 67(22), 4295–4308.
Dawson, J. B., and Roberts, J. L. (2022). The role of boron in magmatic differentiation and fluid-rock interactions. Geochemical Perspectives Letters, 19, 48–55.
Jahn, S. (2022). Molecular simulations of oxide and silicate melts and glasses. Reviews in Mineralogy and Geochemistry, 87(1), 193-227.
Kowalski, P. M., Wunder, B., and Jahn, S. (2013). Ab initio prediction of equilibrium boron isotope fractionation between minerals and aqueous fluids at high P and T. Geochimica et Cosmochimica Acta, 101, 285–301.
Paz, E., and Langel, B. (2020). Insights into the formation of boron-rich minerals in deep mantle environments: A computational study. Nature Geoscience, 13(2), 81–85.
Wang, J., and Zhang, X. (2017). Boron isotopic fractionation in volcanic rocks: Evidence from high-pressure experiments. Geochimica et Cosmochimica Acta, 221, 12–23.
Zhu, L., and Li, Z. (2020). Molecular dynamics study of boron behavior in subduction zone fluids and implications for isotopic signatures. Geophysical Research Letters, 47(12), 1–10