# Thermodynamic Insights into Cubanite and Chalcopyrite Stability in Ni-Cu Sulfide Systems

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## Summary

Cubanite ($CuFe_2S_3$) is an economically significant but metallurgically challenging mineral in magmatic nickel-copper (Ni-Cu) sulfide deposits, where its coexistence with chalcopyrite ($CuFeS_2$) complicates flotation processing. This study, utilizing thermodynamic modeling in FactSage 8.3, demonstrates that cubanite is stable across a broad spectrum of tholeiitic to ferropicritic magmas under reduced conditions, particularly in parental magmas with Ni content below 300 ppm. In contrast, chalcopyrite dominates in tholeiitic magmas with higher Ni concentrations (>300–400 ppm). Our findings indicate that in a parental magma with low Ni content, cubanite and chalcopyrite coexist at R = 1100 across a wide redox range, from ΔQFM > -0.6 in tholeiitic magmas ($Fe_2O_3$ ~9 wt%) to ΔQFM > +0.8 in ferropicritic magmas ($Fe_2O_3$ up to 17 wt%), closely replicating natural sulfide compositions. These results provide a new framework for understanding cubanite stability, enhancing our ability to predict mineral occurrences and optimize extraction strategies for Ni-Cu sulfide deposits.

## Introduction and Methodology

Nickel (Ni) and Copper (Cu) are critical elements for advancing sustainability and enhancing human well-being. These metals are indispensable in modern technologies and pivotal components in green energy solutions. Cubanite ($CuFe_2S_3$), an economically significant yet challenging mineral, is commonly found in magmatic Ni-Cu sulfide deposits. However, its coexistence with chalcopyrite complicates extraction processes in flotation circuits. Understanding the stability conditions of cubanite in magmatic systems (silicate and sulfide melts) is essential for predicting its occurrence in Ni-Cu sulfide deposits and optimizing its extraction.

This study utilizes thermodynamic modeling with FactSage to evaluate the stability of cubanite and chalcopyrite under varying conditions, focusing on oxygen fugacity ($fO_2$), sulfur fugacity ($fS_2$), R-factor, and $Fe_2O_3$* and Ni-Cu content in the magma.

To simulate natural systems, first a system containing 99.857% slag and 0.143% matte by weight was created and cooled to the slag solidus temperature. The slag composition, $fO_2$, $fS_2$, and matte composition were recorded at both the liquidus and slag solidus temperatures. Then a new system created representing a cumulate rock by combining 60% of the liquidus olivine phase, 30% of the liquidus matte phase, and 10% of the liquidus slag melt phase. The exact compositions of these phases at the liquidus temperature were used. The system was then cooled, and the matte composition was recorded at the slag solidus temperature. This configuration represented an olivine orthocumulate with net-textured sulfides.

These procedures were repeated across a grid of compositions, varying $Fe_2O_3$* (total iron oxide expressed as $Fe_2O_3$, ranging from 9 to 17 wt%) to capture a spectrum of magmas from tholeiitic to ferro-picritic compositions. Additionally, a wide range of redox conditions relative to the Quartz-Fayalite-Magnetite (QFM) buffer and Ni and Cu content was explored to evaluate their impact on cubanite and chalcopyrite stability.

## Results

Our study reveals that cubanite stability is primarily controlled by parental magma $Fe_2O_3$* content, Ni concentration, redox conditions, and R-factor. These findings provide a systematic framework for understanding how these parameters influence the prevalence of cubanite and chalcopyrite in magmatic sulfide systems.

At an R-factor of approximately 1100, tholeiitic magmas ($Fe_2O_3$ < ~11 wt%) predominantly produce chalcopyrite at high Ni concentrations (>300–400 ppm) regardless of redox conditions. However, at lower Ni content, both chalcopyrite and cubanite can coexist, with cubanite dominating under reduced conditions (ΔQFM < -0.5) and chalcopyrite becoming more favourable under oxidized conditions.

In contrast, picritic to ferropicritic magmas, irrespective of Ni content, favor cubanite formation under reduced conditions. As oxidation increases, chalcopyrite appears alongside cubanite, though cubanite remains the dominant phase. These results suggest that while picritic-ferropicritic magmas under reduced conditions are the most favorable for cubanite formation, cubanite can still stabilize and become prevalent across a broad range of parental magmas within the tholeiitic-ferropicritic spectrum, provided the conditions remain sufficiently reduced.

Our results further indicate that to achieve a sulfide composition resembling natural magmatic sulfide deposits with Ni and Cu contents of approximately 8% and 4%, the coexistence of cubanite and chalcopyrite extends across a wide redox range, from ΔQFM > -0.6 in tholeiitic magmas ($Fe_2O_3$ ~9 wt%) to ΔQFM > +0.8 in ferropicritic systems ($Fe_2O_3$ up to 17 wt%). Additionally, higher R-factors (e.g., R = 1100) promote cubanite and chalcopyrite paragenesis, whereas lower R-factors (e.g., R = 700) favor cubanite dominance over chalcopyrite.

These findings provide new insights into the formation and distribution of cubanite in natural magmatic Ni-Cu sulfide deposits and have practical implications for mineral exploration and processing strategies. Understanding the stability controls of cubanite and chalcopyrite can aid in predicting ore formation conditions and optimizing sulfide flotation efficiency in mineral processing circuits.