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Algorithmic modifications extending MELTS to calculate subsolidus phase relations

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ABSTRACT

Algorithmic modifications to the MELTS software package are presented in order that calculations of heterogeneous phase equilibria can be performed in the subsolidus. Methods are presented for: (1) selecting an “initial guess assemblage” that satisfies the bulk composition constraints; (2) detecting saturation of new phases (including liquid) in an assemblage; (3) adding and removing phases from the assemblage without adjusting the system bulk composition; and (4) constraining the assemblage to a fixed f_{O_2} . These methods have been added to MELTS, allowing it to calculate heterogeneous phase equilibria with or without liquid, closed or open to O, and with fixed intensive variables (P, T), (P, S), (P, H), or (V, T). Applications include fractional melting calculations, metamorphic phase equilibria, and geophysical models of subsolidus regions of the Earth.