1067-00-2328 **Sandra Jeannette Varela*** (sandyarela@yahoo.com), 587 Cappella Dr., Diamond Springs, CA 95619. *Phase Diagram Calculation via Constrained Optimization.*

Material scientists and engineers rely heavily on the accuracy of phase diagrams in an effort to understand how materials act under given circumstances. We introduce an approach differing from other previously known methods of phase diagram calculation in that we are solving it directly as a constrained optimization problem, using sequential quadratic programming technique implemented in the SNOPT solver of the AMPL package. The method is presented here for the ternary Ca-Li-Na system, though it can be used on any multicomponent multi-phase system, including multiple sublattice case. Comparisons with the commonly used phase diagram calculation software Thermo-Calc are provided.

This work has been completed as a part of the 2010 REU Program at George Mason University funded by the NSF-REU and DOD-ASSURE Programs. (Received September 22, 2010)