MODA

Hypothesis and testing of Datamining Model

1	**PURPOSE OF THE DATAMINING** **DATA-BASE MODEL FOR PARAELECTRIC AND FERROELECTRIC PHASES OF PEROVSKITES**	
1.1	**ASPECT OF THE USER CASE TO BE SIMULATED**	*The first goal is to establish a dataset and functions for Gibbs/Helmholtz energy and chemical potential.* *The second goal is to find the composition and temperature dependence of elastic stiffness and static permittivity in continuous functional to be used in model 2 Phase Field*
1.2	**MATERIAL**	*Perovskite (Ba,Sr)TiO3 ferroelectrics*
1.3	**PUBLICATION ON THIS ONE DATA MINING OPERATION**	S. Lee, C. A. Randall, Zi-Kui Liu, Comprehensive Linkage of Defect and Phase Equilibria through Ferroelectric Transition Behavior in BaTiO3-Based Dielectrics: Part 1. Defect Energies Under Ambient Air Conditions, 91(2008) 1748–1752

2	**THE POSTULATED DATA-BASED MODEL**		
2.1	**POSTULATED EQUATION**	**Equation**	$G_m^{system} = \min\left[f_i G_m^{\phi}(x_i, T)\right]$ $G_m^{\phi} = \sum_i \sum_j y_i^I y_j^{II} G_{i:j}^{o,\phi} + RT(a\sum_i y_i^I \ln y_i^I + b\sum_j y_j^{II} \ln y_j^{II}) + {}^{ex}G_m^{\phi}$. ${}^{ex}G_m^{\phi} = \sum_m y_m^{II} \sum_{i,j>i} y_i^I y_j^I \sum_v L_{i,j}^{v,\phi,I}(y_i^I - y_j^I)^v + \sum_i y_i^I \sum_{m,n>m} y_m^{II} y_n^{II} \sum_v L_{m,n}^{v,\phi,II}(y_m^{II} - y_n^{II})^v$ $+\sum_{i,j}\sum_{m,n} y_i^I y_j^I y_m^{II} y_n^{II} L^{rec}$ $x_i = x_i(y_j)$ *L -adjustable parameters to describe interaction effect among atoms*
		Physical quantities	1. *Molar Gibbs energy of individual phases:* G_m^{ϕ} 2. *x_i-composition, y_j-site fraction* 3. *f_i-phase fraction* 4. *T -temperature, R -gas constant* 5. *L -adjustable parameters to describe interaction effect among atoms* 6. *Formation enthalpy, vibrational entropy, molar volume, activity, etc.*
2.2	**DATABASE USED TO TEST THE HYPOTHESIS**	*CALPHAD*	

3	COMPUTATIONAL DETAIL OF TESTING AGAINST DATA	
3.1	NUMERICAL OPERATIONS	*By evaluating the discrete physical properties from experiments and atomistic simulations, the phenomenological expressions of energy, elastic stiffness and permittivity of paraelectric and ferroelectric phases are extrapolated to entire composition and temperature in the spirit of CALPHAD.* *Least-squares optimization*
3.2	SOFTWARE TOOL	*Thermo-Calc PARROT module*
3.3	MARGIN OF ERROR	*The predicted value of energy has an error in 0.1-10 kJ/mole. It is generated from the compromise among the different errors from measured thermal chemical properties and DFT based calculations.*