**FCCI Phase Field Model**

**System Description**

In this FCCI phase field model, we consider 3 phases i.e. ***α* - Uranium** phase (Phase 1), ***NdAs*** phase (Phase 2) and ***UAs*** phase (Phase 3). We will use the CALPHAD approach to model this phases computationally. In CALPHAD approach the Gibbs energy, (in eV) for individual phases is given by:

(1)

where = Gibbs energy for mechanical mixing.

= Gibbs energy contribution for ideal mixing.

= Excess Gibbs energy part.

**Phase 1 (*α* - Orthorhombic):**

(2)

(3)

(4)

where,

= -8407.734 + 130.955151*T* – 26.9182*TlnT* + 1.25156E-03*T2* – 4.42605E-06*T3* +   
 38568*T-1* (298.15*K* < *T* < 955*K*)

= -22521.8 + 292.121093*T* – 48.66*TlnT* (955*K* < *T* < 3000*K*)

is taken from the *SGTE* database.

= 0.05182 *eV*.

= 0.05182 *eV*.

are assumed because these values are not available in the *SGTE* database.

= 4.17 *eV*

= 2.60 *eV*

are calculated using the DFT calculations.

**Phase 2 (*Nd-As*):**

(5)

(6)

(7)

where,

= -1.57 *eV*

is calculated using the DFT calculations.

**Phase 3 (*UAs*):**

(8)

(9)

(10)

where,

**Gibbs free energy curves**

* **When *Nd* concentration is very low in the system.**

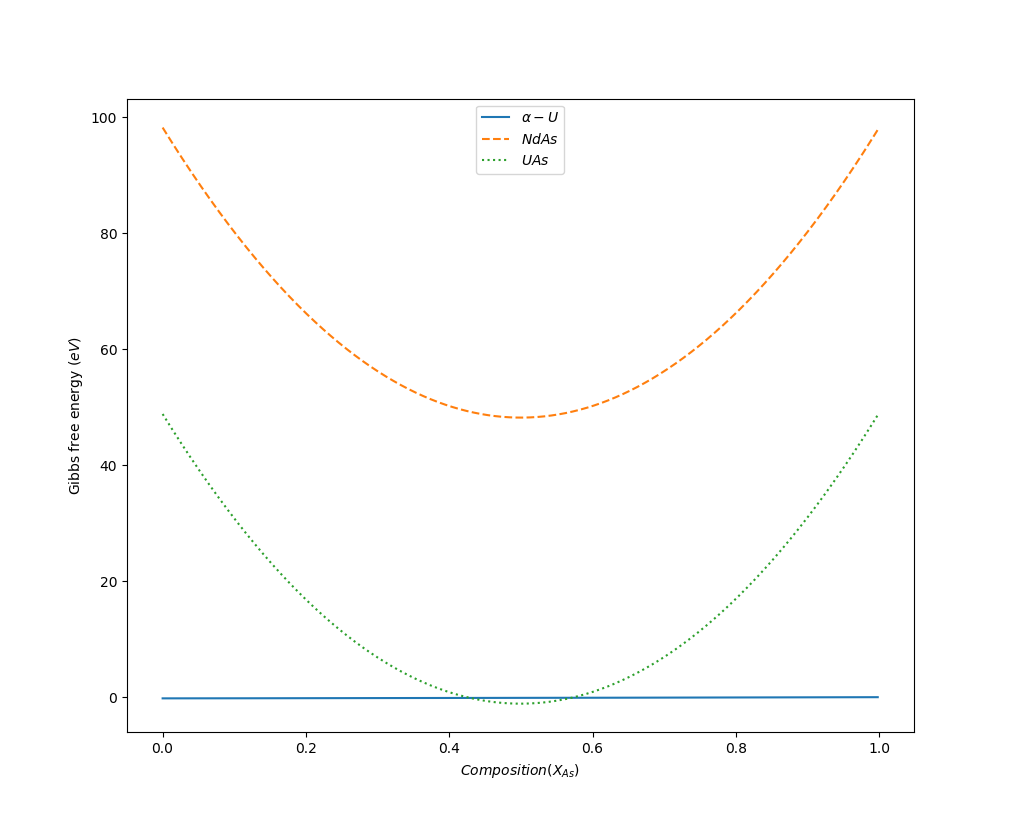
****

Figure 1: Gibbs energy Vs composition curve for the 3 phases in the system at negligible Nd concentration.

* **When *XNd* = *XAs* in the system.**

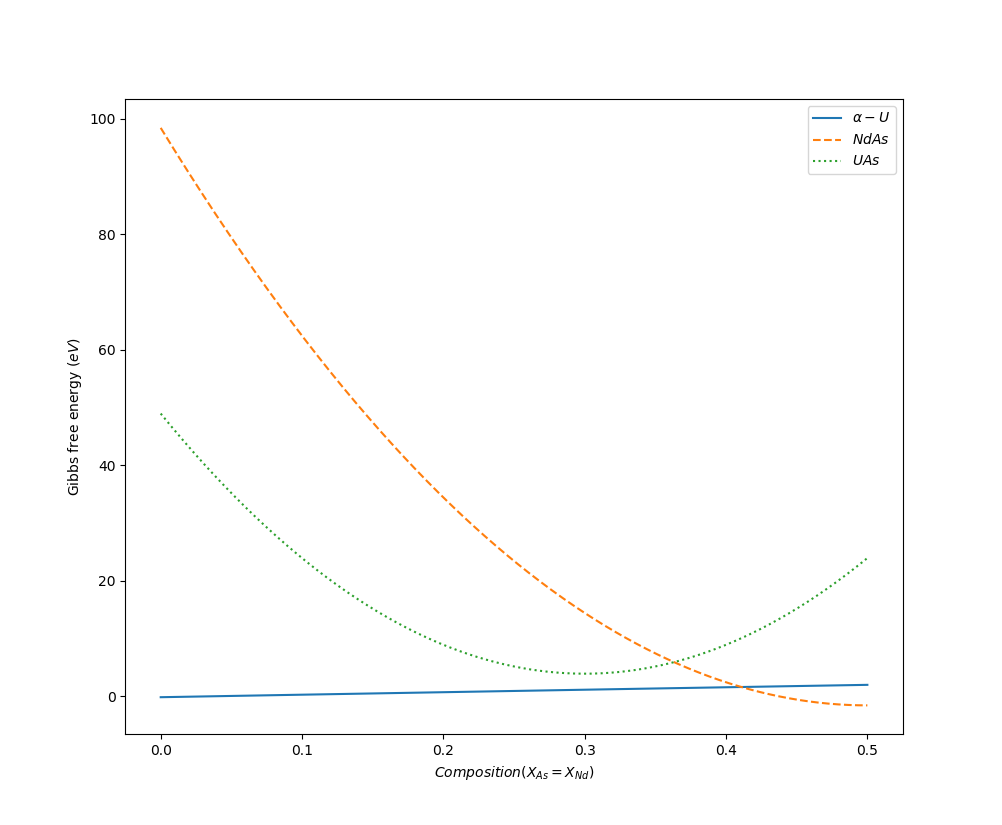
****

Figure 2: Gibbs energy Vs composition curve for the 3 phases in the system at negligible Nd concentration.

**Phase Field Modeling**

We have considered 3 different phases, 2 global and 6 local compositions in the system. This system is modeled with the help of *Kim-Kim-Suzuki* multi-phase field model under the *MOOSE* framework. The *Kim-Kim-Suzuki* multi-phase field model has an advantage over the traditional phase field model as it solves the problem by introducing the concept of phase concentrations. Additionally, in the *Kim-Kim-Suzuki* model, the interfacial width is de-coupled from the interfacial energy and can be changed according to the system requirements without affecting the latter.

For the phase field simulation, we consider a 200 × 1 simulation domain which is scaled from -10 to 10 in the X-axis. The initial values for both the global concentrations viz. *xNd* and *xAs* are taken randomly between 0.2 and 0.21, while all the phase field variables viz. *η1*, *η2* and *η3* have initial values between 0.3 and 0.35. In the simulation, we have considered time step of 10-5 and total end time 107. The results of the phase field simulation at *T* = 300*K* are shown below:

**Initial conditions:**

The initial conditions for the Phase 1, 2 and 3 are taken as smooth hyperbolic tangent which varies from 0 to 1, which represents distinct phases as shown below in the Figure 3 and 4.

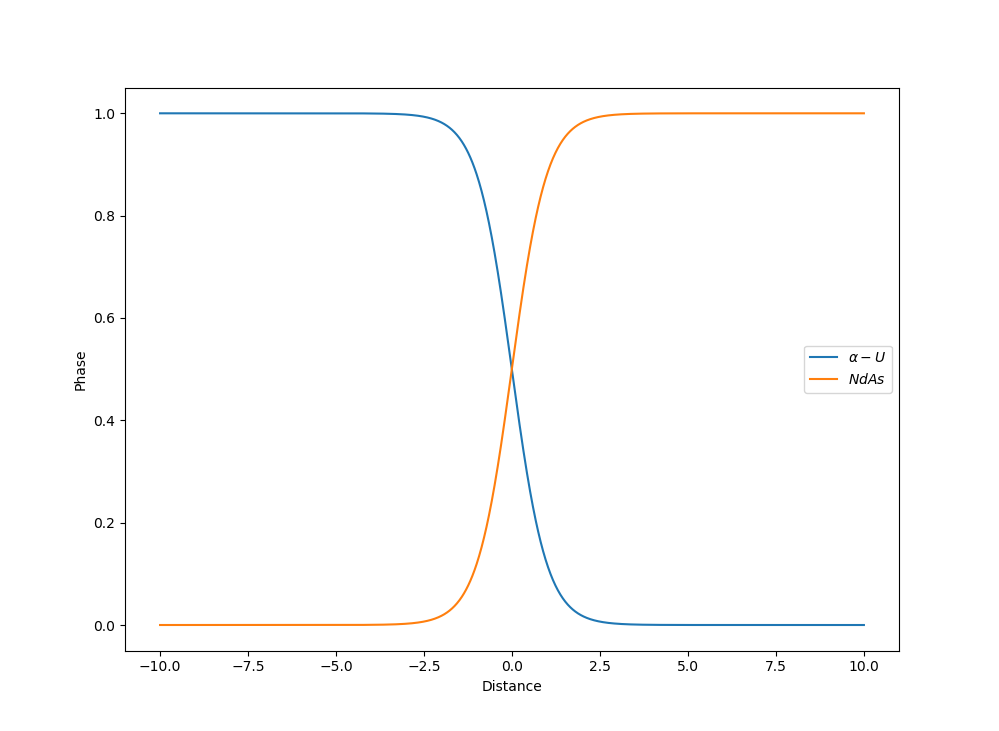


Figure 3: Initial conditions between phase 1 and phase 2 in the phase field simulation.

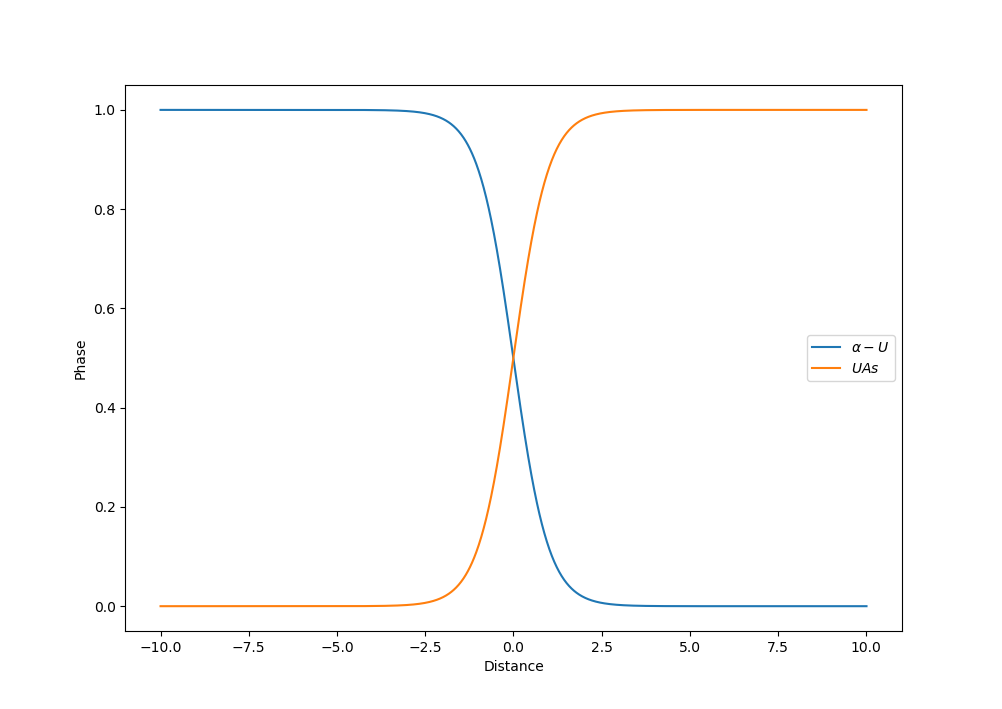
****

Figure 4: Initial conditions between phase 1 and phase 3 in the phase field simulation.

**Simulation results**

**Phase 1 (*α* - Orthorhombic):**

Figure 2: Initial condition (t = 0) of the system with respect to Phase 1.

Figure 3: Intermediate condition (t = 70) of the system with respect to Phase 1.

Figure 4: Final condition (t = 93) of the system with respect to Phase 1.

**Phase 2 (*Nd-As*):**

Figure 5: Initial condition (t = 0) of the system with respect to Phase 2.

Figure 6: Intermediate condition (t = 30) of the system with respect to Phase 2.

Figure 7: Final condition (t = 93) of the system with respect to Phase 2.

**Phase 3 (*UAs*):**

Figure 8: Initial condition (t = 0) of the system with respect to Phase 3.

Figure 9: Intermediate condition (t = 70) of the system with respect to Phase 3.

Figure 10: Final condition (t = 93) of the system with respect to Phase 3.

**Global compositions (*As*)**

Figure 11: Initial condition (t = 0) *xAs*.

Figure 12: Final condition (t = 93) *xAs*.

**Global compositions (*Nd*)**

Figure 13: Initial condition (t = 0) *xNd*.

Figure 14: Final condition (t = 93) *xNd*.

**Discussion**