CALPHAD Description of the Super-cooled Liquid from the Mo-Nb-B System with the 2-State Model

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Abstract

In the present work, we assessed with the CALPHAD method via Thermo-Calc the super-cooled liquid (SCL) that leads to the formation of metallic vitreous materials. This research aimed to improve the database for thermodynamic calculations of SCLs in the computational study of materials, specifically some subsystems of the Fe-Mo-Cr-Nb-B system, since its application as a metallic glass coating combines exceptionally hardness, corrosion resistance and wear resistance. Thus, continuing the work of our group that assessed the Fe-Nb-B system with the same methods and models, we described the liquid Mo with the two-state phenomenological model as well as the binary liquids Mo-Nb and Mo-B.

1. Introduction

The Fe-Nb-B-Mo system is a promising alloy system due to its good amorphous phase-forming ability and to the promotion of high-hardness borides formation. The combination of boride precipitation in an amorphous matrix can form microstructures that combine the good wear resistance properties promoted by borides with the low coefficient of friction and corrosion resistance provided by the amorphous matrix [1-3]. Metallic glasses based on iron have different physicochemical properties than conventional crystalline alloys, for instance, amorphous solids have high corrosion resistance attributed to being chemically more homogeneous and not having crystallographic defects such as grain boundaries, dislocations, and phase boundaries. Therefore, they are less susceptible to chemical attack.

Nevertheless, proper thermodynamical modeling as a key tool for designing amorphous state via CALPHAD method has so far proven to be difficult. Typically, modeling the liquid phase and therefrom the supercooled liquid (SCL) of pure substances has involved a discontinuity of dCp/dT at the melting point, which is not supported by physical evidence and results in unreasonable discontinuities in liquid solutions at the melting points of pure elements. And even though this approach has proven effective in describing crystalline systems, the supercooled liquid Gibbs energy has been only fitted based on
information from low melting binary systems. In this regard, Ågren's two-state liquid is a promising approach for modeling the liquid-amorphous phase in computational thermodynamics [4], as it has a reasonable physical interpretation and shows potential in practical applications. Thus, continuing the work of our group that assessed the Fe-Nb-B liquid system with Ågren's model [5], the assessment of the Mo-Nb-B liquid system is envisioned for a more suitable Fe-Nb-Mo-B database for calculating the properties of SCLs, particularly at large undercoolings. A better thermodynamic description of SCLs can indicate compositional regions with better glass-forming ability (GFA) by analyzing the valleys of the lowest liquidus temperatures in the stable or metastable system by suppressing some slowly crystallizing phases in the calculation. Moreover, the new description allows a more precise calculation of the driving force for crystallization of stable and metastable phases coming from solid amorphous materials compared to current models that thermodynamically describe liquids.

In the present work we assessed through the CALPHAD method the metastable supercooled liquid of the Mo-Nb-B system that leads to the formation of its unstable and "frozen" state known as metallic vitreous material. Specifically, we extended the previous CALPHAD assessment of the Nb-B system done by our group using the two-state model [5] to the ternary Mo-Nb-B. We use Yamada and co-workers [6] assessment of this system as a basis. The assessment procedure is described, and the results are presented.

2. The Mo-Nb-B system

The main difficulty in modeling the Mo-Nb-B liquid system is related to its undercooled region, specifically the difficulty in accurately modeling the amorphous or glass transition. This is due to the lack of adequate experimental data and inherent limitations in fitting models, as typically no low temperature thermodynamic data of the liquid phase are available to determine the model parameters in thermodynamic assessments [7]. The first models for the liquid phase via the CALPHAD method were temperature-dependent expressions, while more recent models also included the contribution of adiabatic heat capacity ($C_p$). These models improve the description of the liquid in temperature ranges where its value is well established (above the melting point, $T_m$), but they may present less satisfactory results for extrapolations below $T_m$, resulting generally in two practical problems: artificial phase stability and the Kauzmann paradox. To address these issues, Dinsdale and co-workers suggested an artificial correction of the liquid and solid heat capacity, where the difference between them is null near 50% below and above $T_m$ [8], which despite solving the two problems mentioned above, it makes the Cp(T) discontinuous and artificial. The second and current generation of SGTE unary databases [9] extrapolates liquid heat capacities below $T_m$ to approach $C_p^{cryst}$ with $\Delta C_p \left( \frac{T}{T_m} \right)^{-9}$ and solid heat capacities above $T_m$ to approach $C_p^L$ with $\Delta C_p \left( \frac{T}{T_m} \right)^7$, which makes the Cp curve less artificial and reduces the two discontinuities proposed by Dinsdale to just one at $T_m$, a comparison between $C_p^{bcc}$ and $C_p^L$ from SGTE are shown in Figure 1. However, this current extrapolation is nonetheless artificial and so forth problematic to model SCLs, thereby Ågren proposed in 1988 a phenomenologically coherent model to represent the thermodynamic properties of the liquid that allows extrapolation to the SCL at low temperatures [4]. The two-state (2st) model proposed by Ågren is based on the phenomenological
hypothesis that atoms present in the SCL can be in a thermodynamic state close to the solid state, that is, only with vibrational degrees of freedom (solid-like atom), or close to the liquid, with vibrational and translational degrees of freedom (liquid-like atom).

This paper does not delve into the details of the 2st model, but instead refers the reader to references [4,10,11] for more information. The model has been shown to provide good agreement with experimental data when applied to other systems such as pure Ga, Au [10], Sn [11], and Fe [12], the binaries Ag-Cu [13] and Fe-B [14], as well as the ternary Fe-Nb-B [5]. In this work, the researchers used the solid phase description for the Mo-Nb-B system provided by Yamada and co-workers [6], and reassessed the CALPHAD description of the liquid phase using Ågren’s 2st liquid model.

2.1. The unary liquid phases

The two-state model describes the molar Gibbs free energy of a pure liquid, $G_m^L$, based on the molar Gibbs energies for the idealized cases of liquid-like and solid-like atoms, $G_m^{liq}$ and $G_m^{sol}$, respectively. $G_m^{liq}$ describes a hypothetical situation where all atoms are in free translation, while $G_m^{sol}$ describes a frozen configuration of the liquid-like state, i.e., an amorphous solid. Assuming a gradual equilibrium transition as a function of temperature, a fraction $\chi$ of atoms will be in the liquid-like state and another $1-\chi$ will be in the solid-like state, so that in the ideal solution model, the Gibbs energy of mixing these two states that describes the 2st liquid is given by:

\[
G_m^L = G_m^{sol} + \chi \Delta G_m^d + RT[(1-\chi)\ln(1-\chi) + \chi \ln \chi]
\]

The parameter $\Delta G_m^d$, which represents the difference in molar Gibbs free energy between the two idealized atom states, is a parameter that needs to be described in the assessment. Similarly, $G_m^{sol}$ is also a parameter that needs to be described and assessed as a function of temperature based on the molar Gibbs free energy of the standard crystal.

The two-state liquid model is built in the Thermo-Calc software which uses the minimum of $G_m^L$ at the equilibrium value of $\chi$ for a given temperature, i.e., it calculates the fraction of internal equilibrium at each temperature by minimizing Equation 1 with the provided $G_m^{sol}$ and $\Delta G_m^d$ descriptions.

Thus, for the pure element B we followed the descriptions of Ref. [14]:

\[
G_m^{sol}(B) = G_B^{\beta} + A^B + B^B T \ln T + C^B T^2 - RT
\]

\[
\Delta G_d(B) = \Delta H_f^B - RT
\]

and for the pure element Nb we followed the descriptions of Ref. [5]:
$G_m^{sol}(Nb) = G_{Nb}^{bcc} + A + CT^2$

$\Delta G_m^{Nb} = \Delta H_f^{Nb} + D - RT$

where $G_i^{phase}$ is the molar Gibbs energy of the standard reference crystal phase of element “i” by Dinsdale [8], $\Delta H_i^f$ is the molar equilibrium crystallization enthalpy of this phase and R is the communal entropy (gas constant) while A, B, C and D are parameters assessed by the respective references. The values of these parameters adopted for pure B and Nb in the liquid phase are presented in Table 1.

There was no previous assessment of liquid Mo in the two-state model. Therefore, given a chosen description for $G_m^{sol}$ and $\Delta G_m^d$ the parameters were assessed using Thermo-calc’s optimization routine PARROT which uses an algorithm of least square method for a given number of experimental data. In the present assessment the researchers used information from the SGTE Ref. [15] on melting point, $T_m^{Mo} = 2896K$, enthalpy change at the melting point, $\Delta H_f^{Mo} = 37480 J/mol$, and heat capacity data close to the melting point, $C_p^{Mo}(T_m) = 42.6 J/K.mol$. It is worth mentioning that in 2018 Minakov and co-workers addressed the Mo properties through ab initio and quantum molecular dynamics (QMD) simulations [16]. They demonstrated that some experimental data can be accurately described by the QMD approach resulting in a slightly smaller enthalpy, $\Delta H_f^{Mo} = 34000 J/mol$, and heat capacity, $C_p^{Mo}(T_m) = 40.7 J/K.mol$. In the solid phase, the first-principles calculations agree perfectly with the Mo density measurements by the electrostatic levitation technique, while for liquid Mo, excellent agreement is achieved with the measurements by the microsecond pulse heating technique. Finally, the authors formulated the enthalpy of the solid and liquid as a function of temperature in their respective stability regions, thus obtaining good agreement between the adiabatic heat capacity calculated for solid and liquid Mo near the melting point and the experimental data. The enthalpy equation for the liquid phase proposed by Minakov is described by Equation 6 and given in $kJ/mol$. We used this equation as a comparative in the choice of $G_m^{sol}$ and $\Delta G_m^d$ descriptions for liquid Mo in the 2-state model.

$\Delta H_f^{Mo}(T) = 31,03034 + 27,04765.10^{-3}T + 2,07981.10^{-6}T^2$

This work tested the descriptions proposed by Alvares for modeling liquid Nb, Equation 2 and Equation 3 [5]; by Ågren for modeling liquid B, Equation 4 and Equation 5 [14]; by Sundman for modeling liquid Fe [16] as well as some mixing variations of these equations. After several assessments via Thermo-Calc’s PARROT with different descriptions and adjustment data (i.e., sometimes adding Minakov’s liquid enthalpy equation), the one with the lowest relative standard deviation to the embedded data, the smallest number of adjustable variables and no thermodynamic inconsistencies (i.e., $C_p^{liq}$ smaller than $C_p^{bcc}$ or $S_m^{liq}$ smaller than $S_m^{bcc}$ at temperatures well below $T_m$) was chosen. The description that best satisfied these conditions was Alvares’ modification with common entropy in $G_m^{sol}$, represented in Equation 7 and Equation 8. The resulting variables of this assessment are shown in Table 1. Figure 1 shows the adiabatic heat capacity of the 2st description for liquid Mo in comparison with other descriptions.
Equation 7

\[ G_m^{\text{sol}}(\text{Mo}) = G_M^{\text{bcc}} + A + CT^2 - RT \]

Equation 8

\[ \Delta G_d^{\text{Mo}} = \Delta H_f^{\text{Mo}} + D - RT \]

Figure 1: Thermal behavior of the \( C_p^{\text{Mo}} \) of the two-state liquid description proposed in this work (black), the liquid (gray), and the BCC solid (dashed gray) from the SGTE database [15], and the liquid studied via QMD by Minakov [16] (red).

2.2. The binary liquid phases

The two-state model extended to solutions uses the regular solution formalism, as described by Equation 9 and Equation 10 for an arbitrary solution between elements A and B.

Equation 9

\[ G_{AB}^{\text{sol}} = x_A^L G_A^{\text{sol}} + x_B^L G_B^{\text{sol}} + x_A^L x_B^L \Delta G_{AB}^{\text{sol}} \]

Equation 10

\[ \Delta G_d^{AB} = x_A^L \Delta G_d^A + x_B^L \Delta G_d^B + x_A^L x_B^L \Delta G_d^{AB} \]
where $L^\text{sol}_{AB}$ and $E \Delta G^A_d$ is described by the Redlich-Kister polynomial, shown in Equation 11, with $k$ interaction parameters, $k^L_{AB}$ [14]. We assume a mechanical mixture of the energy variations between the idealized states of the atoms, $\Delta G^A_d$, setting the excess term $E \Delta G^A_d$ to zero [5,14].

$$L^\text{sol}_{AB} = x_A x_B \sum_{k=0}^{n} k^L_{AB}(x_A - x_B)^k$$

We accepted the assessed interaction parameters for the liquid Nb-B proposed by Alvares [5] who used the temperatures and compositions of all eutectic, peritectic, and congruent melting reactions in the system, obtained from the database of Yoshitomi and co-workers [17]. $E \Delta G^\text{NbB}_d$ was set equal to zero. The first and second-order interaction parameters were described as linearly dependent on temperature, and the third-order parameter was constant. The optimized parameters are presented in Table 1.

The Mo-Nb system presents a complete solubility in their liquid and in their single BCC phase. Since there are no invariant reactions beside the melting points of their pure elements, experimental data about the liquidus and the solidus given by Kocherrzhinskij and Vasilenko in 1981 [18] and by Rudy in 1969 [19] were embedded to optimize several descriptions of parameters. Despite several trials the only description with no inconsistencies in the enthalpy results was the one of the simplest one: two constant interaction parameters. The resulting new binary parameters for the Mo-Nb 2st liquid are presented in Table 1. Figure 2 shows the calculated phase diagram with the 2st liquids and the Yamada description with SGTE liquids.

To assess the two-state liquid thermodynamic description of the Mo-B system, we accepted the solid phases modelling and parameters proposed by Yamada and co-workers where the solid-liquid invariants were considered as experimental data and were embedded at the assessment of the polynomial coefficients [6]. However, given 6 invariant reactions involving the liquid phase to be satisfied and only 4 variables to be assessed in the description proposed by Yamada and co-workers (first-order interaction parameter described as linearly dependent on temperature, the second and third-order parameter, constant), no adequate convergence has been found for the parameters while using the 2st liquid for B and Mo. Nonetheless, when using directly the interaction parameters given by Yamada with the 2st liquids we found a similar phase diagram with the invariant reaction on the same compositions and the temperatures slightly higher compared to the original description which uses the SGTE liquids. Therefore, in order to lower such temperatures, some changes in Yamada's description were manually tested, specifically reducing only the thermal component in the first-order parameter, $L^\text{sol}_{MoB}$, and as a result we obtained a new description that calculates the Mo-B binary diagram with a low deviation compared to the original description given by Yamada (with SGTE liquids). The resulting new binary parameters for the Mo-B 2st liquid are presented in Table 1. Figure 3 presents the calculated Mo-B phase diagram compared with the calculated by Yamada and co-workers.

Table 1 presents all the assessed coefficients for the Mo-Nb-B liquid system, and Table 2 compares the experimental invariant temperatures and compositions calculated by Yamada and co-workers, together with the invariants calculated using the assessed parameters (Table 1).
Table 1: Assessed parameters for the two-state liquid in Mo-Nb-B system (in J/mol formula unit).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_m^{sol,B} = 0G_B^{beta} + 47528.9 - 1.911T\ln T + 0.00197T^2 - RT$</td>
<td>[14]</td>
</tr>
<tr>
<td>$\Delta G_d^B = 50200 - RT$</td>
<td>[14]</td>
</tr>
<tr>
<td>$G_m^{sol,Nb} = 0G_{Nb}^{bcc} + 16826 - 0.00197T^2$</td>
<td>[5]</td>
</tr>
<tr>
<td>$\Delta G_d^{Nb} = 30040 + 8862.3 - RT$</td>
<td>[5]</td>
</tr>
<tr>
<td>$G_m^{sol,Mo} = 0G_{Mo}^{bcc} + 33222.09 - 0.001067T^2 - RT$</td>
<td>This work</td>
</tr>
<tr>
<td>$\Delta G_d^{Mo} = 37500 - 6512.61 - RT$</td>
<td>This work</td>
</tr>
<tr>
<td>$L_{0}^{NbB_{Liq}} = -168126 + 0.28T$</td>
<td>[5]</td>
</tr>
<tr>
<td>$L_{1}^{NbB_{Liq}} = 16048 - 28.1T$</td>
<td>[5]</td>
</tr>
<tr>
<td>$L_{2}^{NbB_{Liq}} = 4623.4$</td>
<td>[5]</td>
</tr>
<tr>
<td>$L_{0}^{MoNB_{Liq}} = -29950.09$</td>
<td>This work</td>
</tr>
<tr>
<td>$L_{1}^{MoNB_{Liq}} = 5967.09$</td>
<td>This work</td>
</tr>
<tr>
<td>$L_{0}^{MoB_{Liq}} = -120000 + 4.1 \times T$</td>
<td>[6] and This work</td>
</tr>
<tr>
<td>$L_{1}^{MoB_{Liq}} = -19000$</td>
<td>[6] and This work</td>
</tr>
<tr>
<td>$L_{2}^{MoB_{Liq}} = +14000$</td>
<td>[6] and This work</td>
</tr>
</tbody>
</table>

Table 2: Comparison of the invariant temperatures in equilibrium with liquid in the binaries. This work, Yamada et al. assessment [6], experimental data. Temperature in K, composition in atom percent.

<table>
<thead>
<tr>
<th>Equilibrium</th>
<th>This work and [5], calculated</th>
<th>Yamada [6], calculated</th>
<th>Experimental or assessed, for comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Nb-B</td>
<td>T (K); at.% B</td>
<td>T (K); at.% B</td>
<td>T (K); at.% B</td>
</tr>
<tr>
<td>$\alpha$-Nb ↔ L</td>
<td>2750; 0</td>
<td>2750; 0</td>
<td>2748 ± 5</td>
</tr>
<tr>
<td>$\beta$B ↔ L</td>
<td>2350; 100</td>
<td>2348; 100</td>
<td>2348 ± 5</td>
</tr>
<tr>
<td>$\alpha$-Nb + NbB ↔ L</td>
<td>2440; 14.3</td>
<td>2440; 15</td>
<td>2438 ± 10; ~16</td>
</tr>
<tr>
<td>NbB ↔ L</td>
<td>3176; 50</td>
<td>3175; 50</td>
<td>3190 ± 10; ~50</td>
</tr>
<tr>
<td>NbB + Nb$_5$B$_6$ ↔ L</td>
<td>3176; 50.6</td>
<td>3175; 52</td>
<td>3133 ± 10, ~52</td>
</tr>
<tr>
<td>Nb$_5$B$_6$ ↔ Nb$_3$B$_4$ + L</td>
<td>3178; 54.5</td>
<td>3195; 54.5</td>
<td>3170 ± 10, ~54</td>
</tr>
</tbody>
</table>
\[
\begin{align*}
\text{Nb}_3\text{B}_4 & \leftrightarrow \text{NbB}_2 + \text{L} & 3190; 57.1 & & 3195; 57 \\
\text{NbB}_2 & \leftrightarrow \text{L} & 3314; 65 & & 3308; 66 & & 3309 \pm 15, \sim 67 & [19] \\
\beta\text{B} + \text{NbB} & \leftrightarrow \text{L} & 2272; 95.7 & & 2277; 95.3 & & 2308 \pm 20, \sim 98 & [19]
\end{align*}
\]

<table>
<thead>
<tr>
<th>System Mo-B</th>
<th>T (K); at.% B (this work)</th>
<th>T (K); at.% B</th>
<th>T (K); at.% B</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha\text{-Mo} \leftrightarrow \text{L})</td>
<td>2896; 0</td>
<td>2896; 0</td>
<td>2892 \pm 5; 0</td>
<td>[20]</td>
</tr>
<tr>
<td>(\alpha\text{-Mo} + \text{Mo}_2\text{B} \leftrightarrow \text{L})</td>
<td>2475; 20.3</td>
<td>2472; 20.3</td>
<td>2448 \pm 6; 23</td>
<td>[19]</td>
</tr>
<tr>
<td>(\text{Mo}_2\text{B} \leftrightarrow \text{L} + \text{MoB})</td>
<td>2550; 27</td>
<td>2550; 27</td>
<td>2553 \pm 12; \sim 33</td>
<td>[19]</td>
</tr>
<tr>
<td>(\text{MoB} \leftrightarrow \text{L})</td>
<td>2884; 50</td>
<td>2885; 50</td>
<td>2873 \pm 8; \sim 50</td>
<td>[19]</td>
</tr>
<tr>
<td>(\text{MoB}_2 \leftrightarrow \text{L} + \text{MoB})</td>
<td>2630; 58</td>
<td>2630; 58</td>
<td>2648 \pm 15; \sim 63</td>
<td>[19]</td>
</tr>
<tr>
<td>(\text{Mo}_2\text{B}_5 \leftrightarrow \text{L} + \text{MoB}_2)</td>
<td>2633; 68</td>
<td>2634; 68</td>
<td>2413 \pm 15; \sim 69</td>
<td>[19]</td>
</tr>
<tr>
<td>(\beta\text{B} + \text{Mo}_2\text{B}_5 \leftrightarrow \text{L})</td>
<td>2180; 88.5</td>
<td>2180; 88.5</td>
<td>2193 \pm 25; 94</td>
<td>[19]</td>
</tr>
</tbody>
</table>

Figure 2: The figure shows a comparison of Nb-Mo phase diagrams using different liquid descriptions. The orange lines represent the phase diagram using the SGTE liquid parameters with binary parameters adjusted by Yamada [6]. The black lines represent the phase diagrams using the two-state liquid model, with the liquid Nb assessed by Alvares [5] and the liquid Mo and the binary parameters assessed from the present work.
2.3. The ternary liquid phase

Due to the scarcity on experimental data of the Mo-Nb-B liquids, Yamada and co-workers [6] proposed a single arbitrary ternary interaction parameter $L_{\text{Mo,Nb,B}}^{\text{Liq}} = -150 \text{ kJ/mol}$ or no ternary interaction parameter $L_{\text{Mo,Nb,B}}^{\text{Liq}} = 0 \text{ kJ/mol}$. We accepted the proposals by Ref. [16] in view of the good agreement of the calculated results for both cases as shown in Figure 5 and Figure 6. The Mo-Nb-B system has no ternary solid phases. The sublattice models for the compounds with homogeneity range proposed by Yamada and co-workers for the solid phases [6] were accepted and are described in Table 3.

Table 3: Sublattice models for compounds with homogeneity range described by Yamada and co-workers [6].

<table>
<thead>
<tr>
<th>Phase</th>
<th>Sublattice Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Mo,Nb)B₂</td>
<td>$\left(\begin{array}{c} Mo_{y_{Mo}^{(1)}}, Nb_{y_{Nb}^{(1)}}, Va_{y_{Va}^{(1)}} \end{array}\right)<em>1 \left(\begin{array}{c} B</em>{y_{B}^{(2)}}, Va_{y_{Va}^{(2)}} \end{array}\right)_2$</td>
</tr>
<tr>
<td>(Mo,Nb)ₓBₓ</td>
<td>$\left(\begin{array}{c} Mo_{y_{Mo}^{(1)}}, Nb_{y_{Nb}^{(1)}} \end{array}\right)<em>X \left(\begin{array}{c} B</em>{y_{B}^{(2)}=1} \end{array}\right)_Y$</td>
</tr>
</tbody>
</table>
3. Results

Considering the stable equilibria there was good agreement in the calculated binary invariants, as presented in Table 2. Calculations with the data of the present assessment reproduced very well the solid-solid relation presented in isotherms published by Yamada and co-workers [6]. The liquidus projection also agreed quite well with Yamada’s [6] as shown in Figure 5 and Figure 6.

Considering the meta-stable equilibria, we expect a difference between the liquid models at large undercoolings, for that matter a metastable phase diagram of the Mo-B system was studied. Figure 4 shows these diagrams which were calculated with no solid phases except the standard stable phase of each element. As expected the difference is noticeable below 1500K where the two-state model calculates a significantly lower composition and metastable eutectic temperature than the SGTE model; moreover the two-state model calculates a significantly smaller metastable solubility range of B in the Mo BCC network (from ~13at.% to ~750K with the SGTE model to ~9at.% to ~600K with the 2st model).

**Figure 4: Superposition of two metastable diagrams of the Mo-B system. The orange lines represent the one calculated with the liquid modeled by SGTE [6] and the blue lines the one calculated with the two-state liquid model assessed by this work.**
Figure 5: Superposed liquidus projections of the Mo-Nb-B system, one calculated with the SGTE liquid model (blue) by Yamada \cite{Yamada6} and the other with the 2st model (orange). Both calculated without the liquid ternary interaction parameter $L_{Mo,Nb,B}^{Liq} = 0 \text{ kJ/mol}$.
4. Conclusion

The Mo-Nb-B system was successfully reassessed using the two-state liquid model proposed by Ågren for the liquid phase and based on the previous assessment of Yamada and co-workers changing only the parameters for the liquid phase. The parameters for the pure element liquid phases were taken directly from previous assessments, indicating the consistency of the model. In the next step of this work, continuing the previous work of Alvares who reassessed the Fe-Nb-B system with the two-state model, we plan to finalize the whole Fe-Mo-Nb-B system with the two-state model which is more suitable for investigating the amorphous alloys of this system.
References


