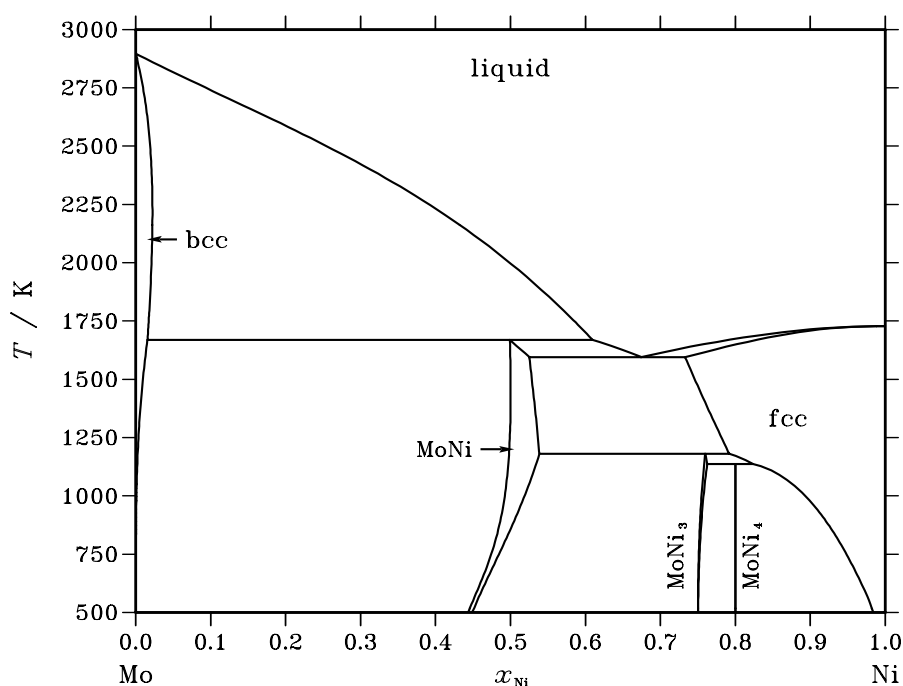


Mo – Ni (Molybdenum – Nickel)**Fig. 1.** Calculated phase diagram for the system Mo-Ni.

Mo and Ni are both alloying elements in steels and other alloys. The solubility of Ni in Mo is small but Ni can dissolve extensive amounts of Mo at high temperature. There are three intermetallics, MoNi₄ which is modelled as stoichiometric, MoNi₃ which is stable in a limited composition range and MoNi which forms peritectically from the liquid and modelled with three sublattices. The assessment has been reported in [99Cui].

Table I. Phases, structures and models.

| Phase | Strukturbericht | Prototype | Pearson symbol | Space group | SGTE name | Model |
|-------------------|-----------------|----------------------------|----------------|--------------|-----------|--|
| liquid | | | | | LIQUID | (Mo,Ni) ₁ |
| bcc | A2 | W | cI2 | $Im\bar{3}m$ | BCC_A2 | (Mo,Ni) ₁ |
| MoNi | ... | ... | oP112 | $P2_12_12_1$ | NIMO | Ni ₆ (Mo,Ni) ₅ Mo ₃ |
| MoNi ₃ | D0 _a | β Cu ₃ Ti | oP8 | $Pm\bar{m}n$ | D0A_NI3X | (Mo,Ni) ₃ (Mo,Ni) ₁ |
| MoNi ₄ | D1 _a | MoNi ₄ | tI10 | $I4/m$ | D1A_NI4X | Ni ₄ Mo ₁ |
| fcc | A1 | Cu | cF4 | $Fm\bar{3}m$ | FCC_A1 | (Mo,Ni) ₁ |

Table II. Invariant reactions.

| Reaction | Type | T / K | Compositions / x_{Ni} | | | | $\Delta_r H$ / (J/mol) |
|--|-------------|--------|-------------------------|-------|-------|--|------------------------|
| bcc + liquid \rightleftharpoons MoNi | peritectic | 1668.3 | 0.016 | 0.610 | 0.499 | | -13290 |
| liquid \rightleftharpoons MoNi + fcc | eutectic | 1595.6 | 0.674 | 0.525 | 0.733 | | -14288 |
| MoNi + fcc \rightleftharpoons MoNi ₃ | peritectoid | 1180.2 | 0.538 | 0.792 | 0.760 | | -4075 |
| MoNi ₃ + fcc \rightleftharpoons MoNi ₄ | peritectoid | 1136.6 | 0.762 | 0.824 | 0.800 | | -2795 |

Table IIIa. Integral quantities for the stable phases at 1800 K.

| Phase | x_{Ni} | ΔG_{m} [J/mol] | ΔH_{m} [J/mol] | ΔS_{m} [J/(mol·K)] | G_{m}^{E} [J/mol] | S_{m}^{E} [J/(mol·K)] | ΔC_P [J/(mol·K)] |
|--------|-----------------|----------------------------------|----------------------------------|--------------------------------------|--------------------------------------|--|-----------------------------|
| bcc | 0.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |
| | 0.018 | −460 | 683 | 0.635 | 903 | −0.122 | −0.052 |
| liquid | 0.569 | −6617 | 7979 | 8.109 | 3613 | 2.426 | −0.261 |
| | 0.600 | −6920 | 6856 | 7.653 | 3152 | 2.058 | −0.243 |
| | 0.700 | −7295 | 3774 | 6.150 | 1847 | 1.071 | −0.182 |
| | 0.800 | −6629 | 1578 | 4.559 | 860 | 0.399 | −0.121 |
| | 0.900 | −4634 | 306 | 2.745 | 231 | 0.042 | −0.061 |
| | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |

Reference states: Mo(bcc), Ni(liquid)

Table IIIb. Partial quantities for Mo in the stable phases at 1800 K.

| Phase | x_{Mo} | ΔG_{Mo} [J/mol] | ΔH_{Mo} [J/mol] | ΔS_{Mo} [J/(mol·K)] | G_{Mo}^{E} [J/mol] | S_{Mo}^{E} [J/(mol·K)] | a_{Mo} | γ_{Mo} |
|--------|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| bcc | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |
| | 0.982 | −257 | 19 | 0.153 | 19 | 0.000 | 0.983 | 1.001 |
| liquid | 0.431 | −257 | 29430 | 16.493 | 12345 | 9.492 | 0.983 | 2.281 |
| | 0.400 | −1859 | 27918 | 16.542 | 11855 | 8.924 | 0.883 | 2.208 |
| | 0.300 | −8103 | 22294 | 16.887 | 9916 | 6.876 | 0.582 | 1.940 |
| | 0.200 | −16708 | 15504 | 17.895 | 7379 | 4.514 | 0.327 | 1.637 |
| | 0.100 | −30299 | 7467 | 20.981 | 4162 | 1.836 | 0.132 | 1.321 |
| | 0.000 | −∞ | −1895 | ∞ | 186 | −1.156 | 0.000 | 1.012 |

Reference state: Mo(bcc)

Table IIIc. Partial quantities for Ni in the stable phases at 1800 K.

| Phase | x_{Ni} | ΔG_{Ni} [J/mol] | ΔH_{Ni} [J/mol] | ΔS_{Ni} [J/(mol·K)] | G_{Ni}^{E} [J/mol] | S_{Ni}^{E} [J/(mol·K)] | a_{Ni} | γ_{Ni} |
|--------|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| bcc | 0.000 | −∞ | 38497 | ∞ | 50551 | −6.697 | 0.000 | 29.303 |
| | 0.018 | −11433 | 36440 | 26.596 | 48495 | −6.697 | 0.466 | 25.541 |
| liquid | 0.569 | −11433 | −8260 | 1.762 | −2997 | −2.924 | 0.466 | 0.819 |
| | 0.600 | −10295 | −7186 | 1.727 | −2650 | −2.520 | 0.503 | 0.838 |
| | 0.700 | −6949 | −4162 | 1.548 | −1611 | −1.417 | 0.629 | 0.898 |
| | 0.800 | −4109 | −1904 | 1.225 | −769 | −0.630 | 0.760 | 0.950 |
| | 0.900 | −1783 | −489 | 0.719 | −206 | −0.158 | 0.888 | 0.986 |
| | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |

Reference state: Ni(liquid)

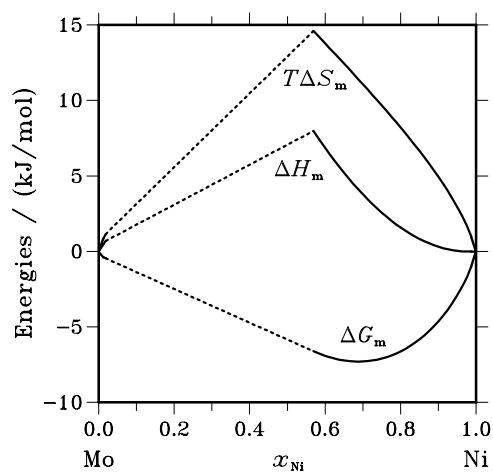


Fig. 2. Integral quantities of the stable phases at $T=1800$ K.

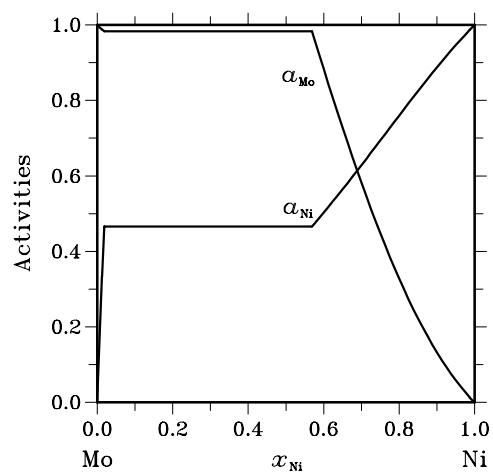


Fig. 3. Activities in the stable phases at $T=1800$ K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

| Compound | x_{Ni} | $\Delta_f G^\circ / (\text{J/mol})$ | $\Delta_f H^\circ / (\text{J/mol})$ | $\Delta_f S^\circ / (\text{J}/(\text{mol}\cdot\text{K}))$ | $\Delta_f C_P^\circ / (\text{J}/(\text{mol}\cdot\text{K}))$ |
|---------------------------------|-----------------|-------------------------------------|-------------------------------------|---|---|
| MoNi ₃ | 0.750 | −2711 | −1984 | 2.441 | 24.708 |
| Mo ₁ Ni ₄ | 0.800 | −2662 | −1883 | 2.612 | −0.612 |

References

- [99Cui] Y. Cui, X. Lu, Z. Jin: Metall. Mater. Trans. A **30A** (1999) 2735–2744.