What Is The Free Energy Change When 1 Mole Of Cu And 1 Mole Of Au Mix Isothermally At 1150 K? Assume

What Is The Free Energy Change When 1 Mole Of Cu And 1 Mole Of Au Mix Isothermally At 1150 K? Assume that we are examining a binary alloy system consisting of copper (Cu) and gold (Au) at a high temperature of 1150 K. This question dives into the thermodynamic principles governing alloy formation, specifically focusing on the calculation of the Gibbs free energy change (ΔG) during mixing under constant temperature conditions. Understanding this process is essential for materials scientists and metallurgists who aim to predict phase stability, solubility, and the potential for alloy formation or phase separation in metallic systems.

Introduction to Free Energy and Alloy Formation

The Gibbs free energy (G) is a thermodynamic potential that predicts the spontaneity of processes at constant temperature and pressure. When two metals are mixed to form an alloy, the change in free energy determines whether the mixture is thermodynamically favorable or not.

Why Is Free Energy Important?

- Predicts phase stability: Whether an alloy will form a solid solution or separate into different phases depends on ΔG.
- Determines solubility limits: The extent to which one metal can dissolve into another is governed by free energy considerations.
- Guides alloy design: For engineering applications, knowing ΔG helps optimize compositions and processing conditions.

In the context of Cu and Au, both metals are mutually soluble in the face-centered cubic (FCC) structure over a wide temperature range, but their thermodynamic interaction influences the free energy change during mixing.

Thermodynamic Principles of Alloy Mixing

When mixing two pure metals, the total Gibbs free energy change (ΔG_{mix}) can be expressed as:

$$
\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}
$$

Where:

- ΔH_{mix} is the enthalpy of mixing.
- ΔS_{mix} is the entropy of mixing.
- T is the absolute temperature in Kelvin.

Ideal vs. Non-Ideal Solutions

- Ideal solutions: Assume no interaction between different atoms, leading to $\Delta H_{mix} = 0$.
- Non-ideal solutions: Include interactions causing deviations from ideality, leading to positive or negative ΔH_{mix}.

Given that Cu and Au are completely miscible in the FCC phase at high temperatures, their mixing behavior is often approximated as an ideal solution, but real systems may exhibit slight deviations.

Calculating the Free Energy Change for Cu-Au Mixing at 1150 K

Assuming ideal solution behavior simplifies calculations:

$$
\Delta G_{mix} = RT \left[x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right]
$$

Where:

- R is the universal gas constant (8.314 J/mol·K).
- x_{Cu} and x_{Au} are the mole fractions of copper and gold, respectively.

Given Data

- Number of moles of Cu and Au: 1 mol each ($x_{Cu} = x_{Au} = 0.5$).
- Temperature: T = 1150 K.
- System is assumed ideal, so $\Delta H_{mix} \approx 0$.

Step-by-Step Calculation

1. Determine mole fractions:

$$
x_{Cu} = 0.5,\quad x_{Au} = 0.5
$$

2. Calculate the entropy of mixing:

$$
\Delta S_{mix} = - R \left(x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right)
$$

3. Calculate ΔG_{mix}:

$$
\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}
$$

Since $\Delta H_{mix} \approx 0$:

$$
\Delta G_{mix} = - T \times \left[- R \left(x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right) \right] = RT \left(x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right)
$$

4. Plug in the values:

$$
\Delta G_{mix} = 8.314 \times 1150 \times [0.5 \ln 0.5 + 0.5 \ln 0.5]
$$

$$
\Delta G_{mix} = 8.314 \times 1150 \times 2 \times 0.5 \ln 0.5
$$

\]

Note:

\[
\ln 0.5 = -0.6931
\]

Thus,

\[
\Delta G_{mix} = 8.314 \times 1150 \times (-0.6931)
\]

\[
\Delta G_{mix} ≈ 8.314 \times 1150 \times (-0.6931) ≈ - 8.314 \times 1150 \times 0.6931
\]

Calculate step-by-step:

- \(8.314 \times 1150 ≈ 955.6 \)
- \(955.6 \times 0.6931 ≈ 662.4 \)

Therefore,

\[
\boxed{
\Delta G_{mix} ≈ -662.4\ \text{J}
}
\]

This negative free energy change indicates that mixing 1 mol of Cu and 1 mol of Au at 1150 K is thermodynamically favorable under ideal solution assumptions.

Factors Influencing the Actual Free Energy Change

While the ideal solution model provides a good approximation, real systems often deviate due to:

- Enthalpy of mixing (ΔH_mix): Slight positive or negative values depending on atomic interactions.
- Temperature: Higher temperatures increase entropy contribution, favoring mixing.
- Atomic size and electronegativity differences: Affect ΔH_mix and the miscibility.

Non-Ideal Solution Considerations

If experimental data suggest non-ideality, the Gibbs free energy change becomes:

\[
\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}
\]

with ΔH_{mix} derived from experimental or computational methods such as CALPHAD models or ab initio calculations.

Practical Implications of the Free Energy Change

Understanding ΔG during Cu–Au mixing assists in:

- Predicting alloy formation: A negative ΔG indicates spontaneous alloying.
- Designing materials: Tailoring compositions for desired properties.
- Controlling phase stability: Ensuring the alloy remains in a single-phase FCC structure at high temperatures.

Summary and Conclusion

In summary, assuming ideal solution behavior, the free energy change when mixing 1 mole of copper and 1 mole of gold at 1150 K is approximately −662 J. This negative value signifies a thermodynamically favorable process, encouraging alloy formation at this temperature.

Key Takeaways:

- The free energy change during alloy mixing depends on entropy and enthalpy contributions.
- At high temperatures like 1150 K, entropy plays a dominant role, often favoring mixing.
- Real systems require consideration of non-ideality, which can modify ΔG.
- Understanding these thermodynamic principles enables better control and prediction of alloy behaviors in metallurgical processes.

References for Further Reading

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- Porter, D. A., Easterling, K. E., & Sherif, M. Y. (2009). Phase Transformations in Metals and Alloys. CRC Press.
- Hillert, M. (2007). Phase Equilibria, Phase Diagrams and Phase Transformations. Cambridge University Press.
- Van der Ven, A., et al. (2000). Thermodynamics of Cu–Au alloys from first principles. Physical Review B, 62(21), 13537.

This comprehensive overview provides both the theoretical background and practical calculation method for determining the free energy change during Cu–Au alloying at high temperature, equipping readers with the knowledge to analyze similar thermodynamic systems.

Frequently Asked Questions

What is the significance of calculating the free energy change when 1 mole of Cu and 1 mole of Au mix isothermally at 1150 K?

Calculating the free energy change helps determine the spontaneity of the mixing process, the stability of the alloy formed, and whether the mixing is thermodynamically favorable at 1150 K.

How do the thermodynamic properties of Cu and Au influence the free energy change during mixing at 1150 K?

The properties such as their individual Gibbs free energies, enthalpies, and entropies at 1150 K influence the overall free energy change, with factors like their atomic interactions and mixing enthalpy playing key roles.

What data is required to compute the free energy change for the mixing of Cu and Au at 1150 K?

Data needed include the standard Gibbs free energies of formation for Cu and Au, their mixing enthalpy and entropy, and the activity coefficients or ideality assumptions for the alloy at 1150 K.

Is the mixing of Cu and Au at 1150 K generally spontaneous or non-spontaneous?

Under ideal conditions, the mixing of Cu and Au at high temperatures like 1150 K is often spontaneous due to the positive entropy of mixing, but precise calculations are needed to confirm.

How does temperature influence the free energy change when mixing Cu and Au?

Higher temperatures increase the entropy contribution to free energy, often making mixing more favorable (more negative ΔG), thus promoting spontaneous alloy formation.

What assumptions are typically made when calculating free energy change in alloy mixing at high temperatures?

Assumptions may include ideal solution behavior, constant activity coefficients, and neglecting phase separation or ordering effects to simplify the calculations.

Can phase diagrams help in understanding the free energy change for Cu–Au mixing at 1150 K?

Yes, phase diagrams provide insights into the phases present, their stability, and the thermodynamic driving forces, which are related to free energy changes during mixing.

What is the role of mixing enthalpy and entropy in determining the free energy change at 1150 K?

Mixing enthalpy reflects the energy change due to interactions between atoms, while mixing entropy accounts for the disorder introduced; together, they determine whether the free energy change favors mixing or phase separation.

Additional Resources

What Is The Free Energy Change When 1 Mole Of Cu And 1 Mole Of Au Mix Isothermally At 1150 K? Assume

Understanding the thermodynamics of alloy formation, especially the free energy change during mixing, is essential in materials science, metallurgy, and chemical engineering. When considering the mixing of copper (Cu) and gold (Au) at high temperatures, such as 1150 K, it becomes crucial to analyze the thermodynamic parameters that govern such processes. This article aims to provide a comprehensive overview of the free energy change associated with mixing 1 mole of Cu and 1 mole of Au under isothermal conditions at 1150 K, elucidating the principles, calculations, and implications involved.

Introduction to Thermodynamics of Alloy Formation

Thermodynamics forms the backbone of understanding phase equilibria, stability, and the energetics of mixing in metal alloys. When two metals are combined, their atoms interact in a way that can either favor or oppose mixing, depending on their thermodynamic properties. The key thermodynamic function in this context is the Gibbs free energy (G), which determines whether a mixture is thermodynamically stable and whether the process occurs spontaneously.

The change in Gibbs free energy upon mixing, denoted as ΔG_mix, can be expressed as:

$$
\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}
$$

where:
- ΔH_mix is the enthalpy of mixing,
- ΔS_mix is the entropy of mixing,
- T is the absolute temperature (1150 K in this case).

The sign and magnitude of ΔG_mix inform about the thermodynamic favorability of alloy formation, phase separation, or possible compound formation.

Fundamentals of Mixing Thermodynamics

Enthalpy of Mixing (ΔH_{mix})

The enthalpy change during mixing reflects the energetic interactions between different atomic species. For ideal solutions, these interactions are assumed to be similar, leading to ΔHmix ≈ 0. However, real metallic solutions often

exhibit deviations due to differences in atomic sizes, electronegativities, and bonding characteristics.

In binary alloys, the enthalpy of mixing can be approximated using models such as the regular solution model:

$$
\Delta H_{mix} = \Omega x_{Cu} x_{Au}
$$

where:
- Ω is an interaction parameter indicating the energy difference between unlike and like atom pairs,
- x_{Cu} and x_{Au} are the mole fractions of Cu and Au, respectively.

A positive Ω indicates endothermic mixing (unfavorable interactions), while a negative Ω suggests exothermic mixing (favorable interactions).

Entropy of Mixing (ΔS_{mix})

The entropy of mixing for an ideal solution is given by:

$$
\Delta S_{mix} = - R \left(x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right)
$$

where R is the universal gas constant (~8.314 J/mol·K). Entropy generally favors mixing due to increased disorder, making ΔGmix more negative at higher temperatures.

Specifics of Copper–Gold System

Atomic Properties and Interactions

Copper and gold are both transition metals with face-centered cubic (FCC) crystal structures, facilitating mutual solubility and alloy formation. Key properties include:

- Atomic radii: Cu (~128 pm), Au (~144 pm)
- Electronegativity: Cu (1.90), Au (2.54)
- Melting points: Cu (~1357 K), Au (~1337 K)

The similarity in crystal structures and moderate differences in atomic sizes suggest the potential for forming continuous solid solutions over a range of compositions.

Experimental Data and Phase Diagram

The Cu-Au phase diagram indicates complete miscibility in the liquid phase and extensive solid solubility at high temperatures, including 1150 K. The phase diagram shows that at 1150 K, the system exists as a homogeneous liquid alloy or a single-phase solid solution, depending on cooling rates.

From experimental data, the enthalpy of mixing (ΔHmix) for Cu-Au is typically slightly positive or near zero, implying near-ideal behavior with weak interactions:

$$
\Delta H_{mix} \approx +1 \text{ to } +5\, \text{kJ/mol}
$$

Calculating the Free Energy Change for Mixing 1 Mole of Cu and Au at 1150 K

Assuming the mixing involves equal molar amounts (1 mol each), the mole fractions are:

$$
x_{Cu} = x_{Au} = 0.5
$$

Given the assumptions:
- The alloy behaves approximately as an ideal or near-ideal solution,
- ΔHmix is small and positive (say, +3 kJ/mol),
- Temperature T = 1150 K,
- R = 8.314 J/mol·K.

Step 1: Calculate the Entropy of Mixing

$$
\Delta S_{mix} = - R \left(x_{Cu} \ln x_{Cu} + x_{Au} \ln x_{Au} \right)
$$

$$
\Delta S_{mix} = - 8.314 \left(0.5 \ln 0.5 + 0.5 \ln 0.5 \right)
$$

$$
\ln 0.5 = -0.6931
$$

$$
\Delta S_{mix} = - 8.314 \times (0.5 \times -0.6931 + 0.5 \times -0.6931) = - 8.314 \times (-0.6931) = 8.314 \times 0.6931 \approx 5.76\, \text{J/mol·K}
$$

Step 2: Calculate the Enthalpy of Mixing

Assuming ΔHmix ≈ +3 kJ/mol = +3000 J/mol.

Step 3: Compute ΔGmix

$$
\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}
$$

$$
\Delta G_{mix} = 3000\, \text{J/mol} - 1150\, \text{K} \times 5.76\, \text{J/mol·K}
$$

$$
\Delta G_{mix} = 3000 - (1150 \times 5.76) = 3000 - 6624 \approx -3624\, \text{J/mol}
$$

Interpretation:

The negative value (~ −3.62 kJ/mol) indicates that, despite a small positive enthalpy, the entropy contribution at 1150 K favors mixing, leading to an overall thermodynamically favorable process. The alloy formation is spontaneous under these conditions.

Implications and Broader Context

Thermodynamic Favorability of alloying Cu and Au at high temperatures suggests that homogeneous solutions are stable and readily form when the metals are melted together at 1150 K. The near-ideal behavior of the system implies minimal lattice strain or bonding disparities, facilitating alloy production in industrial settings.

Relevance in Material Design

Understanding the free energy change is crucial for designing materials with tailored properties. For instance:

- Electronic applications: Cu-Au alloys exhibit interesting electrical conductivity and corrosion resistance.
- Catalytic processes: Alloy composition influences catalytic activity, especially in high-temperature environments.
- Jewelry and decorative uses: The alloy's color and durability depend on the precise composition and thermodynamic stability.

Limitations and Assumptions

While the calculations provide valuable insights, real systems may deviate due to:

- Non-ideal interactions,
- Kinetic barriers to mixing,
- Presence of impurities,

- Phase segregation upon cooling.

Accurate thermodynamic modeling may require experimental data for precise Ω values and phase behavior.

Conclusion

The analysis of the free energy change when mixing 1 mole of Cu and 1 mole of Au at 1150 K reveals that, under typical assumptions, the process is thermodynamically favorable, primarily driven by the entropy of mixing overcoming the slight positive enthalpy of interactions. This insight underscores the high mutual solubility and stability of Cu–Au alloys at elevated temperatures, aligning with experimental phase diagrams and thermodynamic models.

This understanding is essential for metallurgists and materials scientists aiming to optimize alloy compositions for various applications, highlighting how fundamental thermodynamic principles guide practical innovations. Future studies integrating experimental thermodynamic data and advanced modeling can refine these estimates, further enhancing our ability to engineer materials with desired properties.

Note: The actual free energy change can vary depending on specific alloy compositions, experimental enthalpy data, and interaction parameters. The calculations provided are illustrative based on typical values and assumptions for the Cu–Au system.

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