Calculate The Number Of Vacancies Per Cubic Meter In Gold At900C. The Energy For Vacancy Formation Is

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Understanding the behavior of vacancies in metals like gold at elevated temperatures is essential for applications in materials science, metallurgy, and industrial processes. Vacancies—empty atomic sites within a crystal lattice—play a pivotal role in diffusion, mechanical strength, and thermal properties. Specifically, calculating the number of vacancies per cubic meter in gold at 900°C provides insights into the material's structural stability and diffusion characteristics under high-temperature conditions. In this article, we delve into the methodology of calculating vacancy concentration, explore the significance of vacancy formation energy, and demonstrate how to determine the number of vacancies per cubic meter in gold at 900°C.

Fundamentals of Vacancy Formation in Metals

What Are Vacancies?

Vacancies are point defects within a crystal structure where an atom is missing from its lattice site. These defects are inherently present due to thermal agitation and can be thermally generated or introduced during manufacturing processes. Their concentration depends on temperature, the energy needed to form a vacancy, and the entropic factors associated with defect formation.

The Role of Vacancy Formation Energy

The vacancy formation energy, often denoted as Q_v, is the energy required to create a single vacancy in the crystal lattice. This energy barrier influences how many vacancies form at a given temperature. Generally, the higher the vacancy formation energy, the fewer vacancies are generated at a specific temperature.

Calculating Vacancy Concentration in Gold at 900°C

The process involves applying thermodynamic principles, specifically the Arrhenius equation, which relates the vacancy concentration to temperature and vacancy formation energy.

Step 1: Understanding the Theoretical Framework

The equilibrium concentration of vacancies, C_v, in a crystal can be described by the equation:

$$
C_v = N \exp\left(-\frac{Q_v}{k T}\right)
$$

Where:
- C_v is the number of vacancies per atom,
- N is the total number of atomic sites per unit volume,
- Q_v is the vacancy formation energy,
- k is Boltzmann's constant ($1.38 \times 10^{-23} \, \text{J/K}$),
- T is the absolute temperature in Kelvin.

This equation indicates that vacancy concentration exponentially increases with temperature and inversely with the vacancy formation energy.

Step 2: Gathering Necessary Data

To perform the calculation, we need:

- The vacancy formation energy for gold (Q_v),
- The temperature in Kelvin,
- The atomic density of gold (N),
- Boltzmann's constant.

Typical values for gold:

- Vacancy formation energy, Q_v: approximately 1.2 eV (which is $1.2 \times 1.602 \times 10^{-19} \, \text{J} \approx 1.922 \times 10^{-19} \, \text{J}$),
- Melting point of gold: 1064°C, but we're working at 900°C,
- Atomic radius of gold: approximately 144 pm,
- Density of gold: 19.32 g/cm³,
- Atomic weight of gold: 197 g/mol.

Step 3: Calculating Atomic Density N

Number of atoms per unit volume:

$$
N = \frac{\text{Density} \times N_A}{\text{Atomic weight}}
$$

Where:

- N_A is Avogadro's number ($6.022 \times 10^{23} \, \text{atoms/mol}$),
- Density in g/cm³.

Calculating:

$$
N = \frac{19.32 \, \text{g/cm}^3 \times 6.022 \times 10^{23} \, \text{atoms/mol}}{197 \, \text{g/mol}}
\approx 5.9 \times 10^{22} \, \text{atoms/cm}^3
$$

\]

Converting to atoms per cubic meter:

\[
1 \, \text{cm}^3 = 1 \times 10^{-6} \, \text{m}^3
\]

Thus,

\[
N \approx 5.9 \times 10^{22} \times 10^{6} = 5.9 \times 10^{28} \, \text{atoms/m}^3
\]

Step 4: Computing \(C_v \) at 900°C
Convert 900°C to Kelvin:

\[
T = 900 + 273.15 = 1173.15 \, \text{K}
\]

Calculate the exponential term:

\[
\frac{Q_v}{k T} = \frac{1.922 \times 10^{-19}}{1.38 \times 10^{-23} \times 1173.15} \approx \frac{1.922 \times 10^{-19}}{1.620 \times 10^{-20}} \approx 11.86
\]

Therefore,

\[

$$
C_v = N \times \exp(-11.86) \approx 5.9 \times 10^{28} \times 7.0 \times 10^{-6} \approx 4.1 \times 10^{23} \, \text{vacancies/m}^3
$$

This indicates approximately 4.1×10^{23} vacancies per cubic meter in gold at 900°C.

Implications of Vacancy Concentration in Gold

Material Properties and Diffusion

The high vacancy concentration at elevated temperatures significantly influences diffusion processes in gold. Diffusion rates are directly proportional to the vacancy concentration; thus, at 900°C, gold exhibits increased atomic mobility, affecting processes like annealing, alloying, or corrosion.

Mechanical Strength and Creep

Vacancies facilitate dislocation movement, which impacts the mechanical strength of gold. Elevated vacancy levels can lead to softening or creep under stress, especially at high temperatures.

Factors Affecting Vacancy Concentration

Vacancy Formation Energy Variations

While the typical Q_v for gold is around 1.2 eV, impurities, alloying elements, or different crystal structures can alter this energy, affecting vacancy concentrations.

Temperature Dependence

Higher temperatures exponentially increase vacancy concentration, emphasizing the importance of precise temperature control in high-temperature applications.

Material Purity and Defect Interactions

Impurities can act as vacancy traps or sources, modifying the effective vacancy concentration beyond simple thermodynamic calculations.

Conclusion

Calculating the number of vacancies per cubic meter in gold at 900°C involves understanding the thermodynamics of defect formation, gathering accurate material data, and applying the Arrhenius equation. With an approximate vacancy formation energy of 1.2 eV, the vacancy concentration in gold at 900°C is on the order of 4×10^{23} vacancies per cubic meter. This high vacancy density underscores the significant atomic mobility and potential for diffusion-driven phenomena in gold at elevated temperatures. Recognizing these factors is crucial for optimizing high-temperature processes, ensuring material stability, and designing gold-based components for industrial applications.

Keywords: vacancy concentration in gold, vacancy formation energy, high-temperature diffusion, thermodynamics of defects, gold at 900°C, atomic vacancies, materials science, diffusion in metals

Frequently Asked Questions

How do you calculate the number of vacancies per cubic meter in gold

at 900°C?

To calculate the vacancy concentration, use the formula n = N exp(-Qv / (k T)), where N is the atomic density, Qv is the vacancy formation energy, k is Boltzmann's constant, and T is the temperature in Kelvin. Then multiply by the atomic volume to find vacancies per cubic meter.

What is the significance of vacancy formation energy in determining vacancies in gold at high temperatures?

The vacancy formation energy (Qv) determines how easily vacancies form; lower Qv increases vacancy concentration at a given temperature, affecting the material's properties like diffusion and mechanical strength.

What is the typical energy required for vacancy formation in gold at elevated temperatures such as 900°C?

The vacancy formation energy for gold is approximately 1.2 eV, but it can vary slightly depending on specific conditions; this value is used to estimate vacancy concentrations at high temperatures like 900°C.

How does temperature influence the number of vacancies per cubic meter in gold?

As temperature increases, the exponential term in the vacancy concentration formula increases, leading to a higher number of vacancies per cubic meter due to enhanced atomic mobility and vacancy formation.

Why is understanding vacancy concentration important in the context of gold's high-temperature behavior?

Vacancy concentration influences diffusion, mechanical properties, and creep behavior at high temperatures, making it critical for predicting gold's performance in high-temperature applications.

Additional Resources

Calculate The Number Of Vacancies Per Cubic Meter In Gold At 900°C. The Energy For Vacancy Formation Is

Understanding the microscopic properties of metals like gold, especially at elevated temperatures, is essential for advancing fields such as materials science, metallurgy, and nanotechnology. One critical aspect of these properties involves the formation and behavior of vacancies—empty atomic sites within the crystal lattice—that influence diffusion, mechanical strength, and other physical characteristics. This article offers a comprehensive analysis of how to calculate the number of vacancies per cubic meter in gold at 900°C, focusing on the vacancy formation energy and the underlying thermodynamic principles.

Introduction to Vacancies in Metals

Vacancies are intrinsic point defects in crystalline materials, representing the absence of an atom at a lattice site that would normally be occupied in a perfect crystal. Their presence is thermally activated, meaning that as temperature increases, the equilibrium concentration of vacancies also rises. This phenomenon significantly impacts the physical properties of metals, including diffusion rates, creep resistance, and electrical conductivity.

In face-centered cubic (FCC) metals like gold, the behavior and concentration of vacancies are well-studied topics. Their formation energy, which is the energy required to create a vacancy, is a key parameter that influences how many vacancies exist at a given temperature.

Fundamental Concepts and Theoretical Framework

Vacancy Formation Energy (E_f)

The vacancy formation energy, denoted as E_f, is the energy needed to create a vacancy in the crystal lattice. For gold, this value has been experimentally and theoretically determined to be approximately 1.2 eV, although some studies suggest values around 1.0–1.3 eV. This energy barrier influences the equilibrium vacancy concentration at any temperature.

Equilibrium Vacancy Concentration

The number of vacancies per atom at thermal equilibrium, C_v, follows Arrhenius-type behavior:

$$
C_v = \exp\left(-\frac{E_f}{k_B T}\right)
$$

where:

- C_v is the ratio of vacancies to total lattice sites,
- E_f is the vacancy formation energy,
- k_B is Boltzmann's constant (8.617333×10^{-5} eV/K),
- T is the absolute temperature in Kelvin.

This expression indicates that vacancy concentration increases exponentially with temperature.

Converting Vacancy Concentration to Number Density

To find the number of vacancies per unit volume, we multiply the vacancy concentration by the atomic number density:

$$
N_v = C_v \times N_{atoms}
$$

where:
- N_{atoms} is the number of atoms per cubic meter in the perfect crystal lattice.

This approach provides a direct way to estimate vacancies per volume, which is vital for understanding diffusion and mechanical properties.

Step-by-Step Calculation of Vacancy Density in Gold at 900°C

1. Gather Material Parameters

Let's list the parameters needed:

- Temperature (T): 900°C, which converts to Kelvin as:

$$
T = 900 + 273.15 = 1173.15\, \text{K}
$$

- Vacancy formation energy (E_f): For gold, approximately 1.2 eV.

- Atomic weight of gold (Au): 197 g/mol.

- Density of gold (ρ): 19,320 kg/m³.

- Avogadro's number (N_A): 6.022×10^{23} atoms/mol.

- Boltzmann's constant (k_B): 8.617333×10^{-5} eV/K.

---

2. Calculate Atomic Number Density (N_{atoms})

The atomic number density is calculated as:

$$
N_{atoms} = \frac{\text{Number of atoms per mol}}{\text{Volume per mol}}
$$

But more straightforwardly:

$$
N_{atoms} = \frac{\rho}{M} \times N_A
$$

where:

- ρ = mass density of gold = 19,320 kg/m³,
- M = molar mass = 0.197 kg/mol.

Therefore:

$$
N_{atoms} = \frac{19,320\, \text{kg/m}^3}{0.197\, \text{kg/mol}} \times 6.022 \times 10^{23}\, \text{atoms/mol}
$$

Calculating:

$$
\frac{19,320}{0.197} \approx 98,058\, \text{mol/m}^3
$$

So:

$$
N_{atoms} \approx 98,058 \times 6.022 \times 10^{23} \approx 5.9 \times 10^{28}\, \text{atoms/m}^3
$$

---

3. Compute Vacancy Concentration (C_v)

Using the Arrhenius equation:

$$
C_v = \exp\left(-\frac{E_f}{k_B T}\right)
$$

Plugging in the values:

$$
C_v = \exp\left(-\frac{1.2\, \text{eV}}{8.617333 \times 10^{-5}\, \text{eV/K} \times 1173.15\, \text{K}}\right)
$$

Calculate denominator:

$$
8.617333 \times 10^{-5} \times 1173.15 \approx 0.1012\, \text{eV}
$$

Then:

$$
C_v = \exp\left(-\frac{1.2}{0.1012}\right) = \exp(-11.86) \approx 7.1 \times 10^{-6}
$$

This indicates that roughly 7.1 parts per million of lattice sites are vacant at 900°C.

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4. Determine the Number of Vacancies per Cubic Meter (N_v)

Multiplying vacancy concentration by atomic number density:

$$
N_v = C_v \times N_{atoms} \approx 7.1 \times 10^{-6} \times 5.9 \times 10^{28} \approx 4.19 \times 10^{23}\, \text{vacancies/m}^3
$$

Result: Approximately 4.2×10^{23} vacancies per cubic meter exist in gold at 900°C.

Implications and Significance of Vacancy Concentration

Understanding this vacancy density is pivotal for multiple reasons:

- Diffusion: Vacancies serve as vehicles for atomic diffusion. The higher the vacancy concentration, the faster atoms can migrate, influencing processes such as alloying, sintering, and creep.

- Mechanical Properties: Vacancy concentration impacts the strength and ductility of gold. Elevated vacancy levels at high temperatures can lead to softening or enhanced creep behavior.

- Material Stability: Knowledge of vacancy populations guides the design of gold-based components subjected to high-temperature environments, ensuring longevity and reliability.

- Thermal Treatments: This calculation informs thermal processing strategies, such as annealing schedules, to control defect populations.

Factors Affecting Vacancy Concentrations in Gold

While the above calculations provide a theoretical estimate, real-world vacancy concentrations can vary due to:

- Impurities and Alloying Elements: These can either stabilize or destabilize vacancies, altering their equilibrium concentration.

- Non-Equilibrium Conditions: Rapid cooling or mechanical deformation can trap vacancies, leading to non-equilibrium populations.

- Surface and Grain Boundary Effects: Surfaces and grain boundaries act as vacancy sinks or sources, impacting overall vacancy density.

- External Stress and Pressure: Mechanical stresses can influence vacancy formation energies, either promoting or inhibiting vacancy creation.

Advanced Considerations and Refinements

For more precise modeling, several factors might be incorporated:

- Temperature-Dependent Vacancy Formation Energy: E_f can vary with temperature, especially near melting points.

- Vacancy-Vacancy Interactions: At high concentrations, interactions among vacancies can alter their thermodynamic behavior.

- Lattice Vibrations: Phonon contributions at elevated temperatures influence vacancy formation energies.

- Kinetic Factors: The rate of vacancy creation and annihilation depends on diffusion rates and defect migration energies.

In computational materials science, techniques like molecular dynamics simulations and density functional theory (DFT) calculations help refine these estimates.

Conclusion

The calculation of vacancy density in gold at 900°C underscores the profound interplay between thermodynamics and materials properties. With an approximate vacancy concentration of 7×10^{-6}, translating to about 4.2×10^{23} vacancies per cubic meter, it becomes evident that high-temperature environments significantly alter defect populations within the metal lattice. These insights not only deepen our fundamental understanding of gold's behavior under thermal stress but also inform practical applications ranging from electronics to jewelry manufacturing, where high-temperature stability and mechanical integrity are paramount.

By integrating thermodynamic principles with precise material parameters, scientists and engineers can better predict material performance and tailor processing conditions to optimize properties.

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