Vacancy Nature of the bcc Phase in Solid Helium

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Motivation

- The bcc phase is unique one for Rare Gas Solids
- There is strong isotopic effect on bcc phase in solid helium
- Vacancy concentration jump was found under hcp-bcc transition

The main goal

Is to make qualitative model of the bcc phase existence in solid helium:

1. to propose vacancy criteria for both ^{3}He and ^{4}He at pre-melting temperatures;

2. to propose quantum criteria for ^{3}He at low temperatures.

Introduction and Prehistory

Vacancy model

M.E.R. Bernier and J.H. Hetherington. Phys. Rev. B, 39, 16, 11285 (1989)

$$\rho(E) = \begin{cases} \frac{(E-Q_V)^2}{Q_V^3}, & E \geq Q_V \\ 0, & E < Q_V \end{cases}$$ - The density of the states of the vacancies

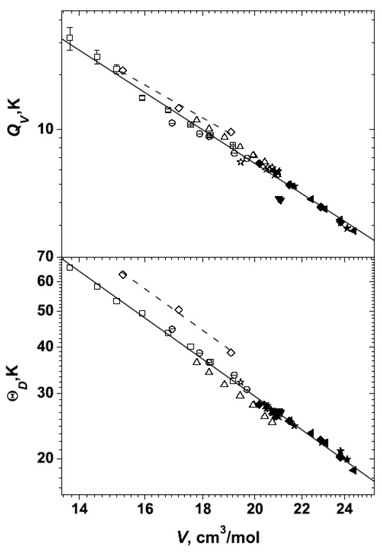
$$x_v = \left(\frac{T}{Q_V}\right)^3 \exp\left[-\frac{Q_V}{T}\right]$$ - The equilibrium vacancy concentration

Contributions to the specific heat:

$$C = \frac{12\pi^4}{5} R\left(\frac{T}{\Theta_D}\right)^3 + R\left(\frac{T}{Q_V} + 6\frac{T^2}{Q_V^2} + 12\frac{T^3}{Q_V^3}\right)\exp\left[-\frac{Q_V}{T}\right]$$

Vacancy and Phonon contributions

V.N. Grigor'ev and Ye.O. Vekhov. J Low Temp Phys 149, 41 (2007)



Closed symbols – the bcc phase of ^{3}He and ^{4}He

Empty symbols – the hcp phase of ^{3}He and ^{4}He

Bcc ^{3}He and hcp ^{4}He

$$\lg Q_V = 6,036 - 4,01_3 \cdot \lg V,$$

$$\lg \Theta_D = 4,30 - 2,17_8 \cdot \lg V,$$

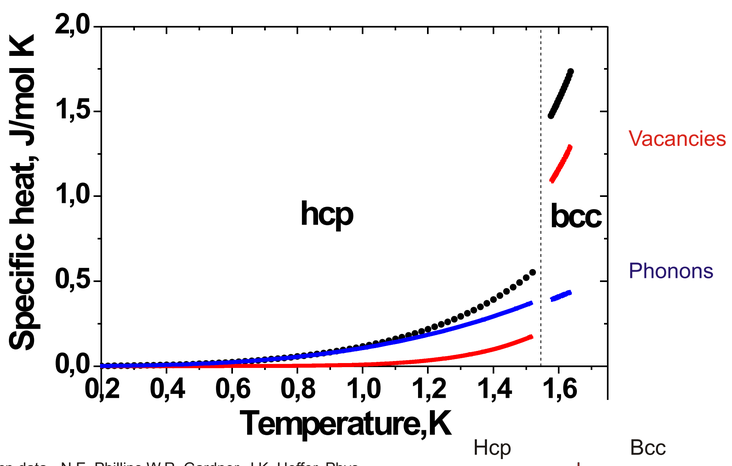
hcp ^{3}He

$$\lg Q_V = 5,513 - 3,54_5 \cdot \lg V,$$

$$\lg \Theta_D = 4,403 - 2,19_6 \cdot \lg V.$$

(a) The vacancy activation energy Q_V and (b) the Debye temperature for solid helium as a function of molar volume on log–log scale.

Specific heat jump under hcp-bcc transition in ^{4}He



Hcp data - N.E. Phillips W.R. Gardner, J.K. Hoffer, Phys. Rev. A. (1973)

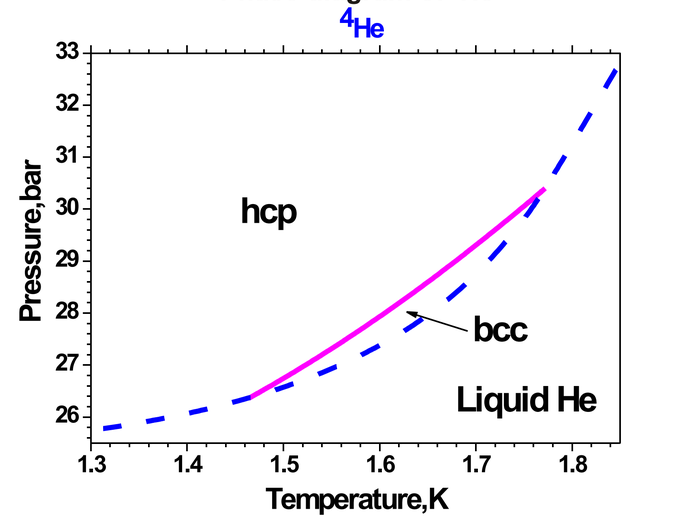
Bcc data - J.K. Hoffer, W.R. Gardner, C.G. Waterfield, N.F. Phillips, JLTP (1976)

Analysis - V.N. Grigor'ev and Ye.O. Vekhov. J Low Temp Phys 149, 41 (2007)

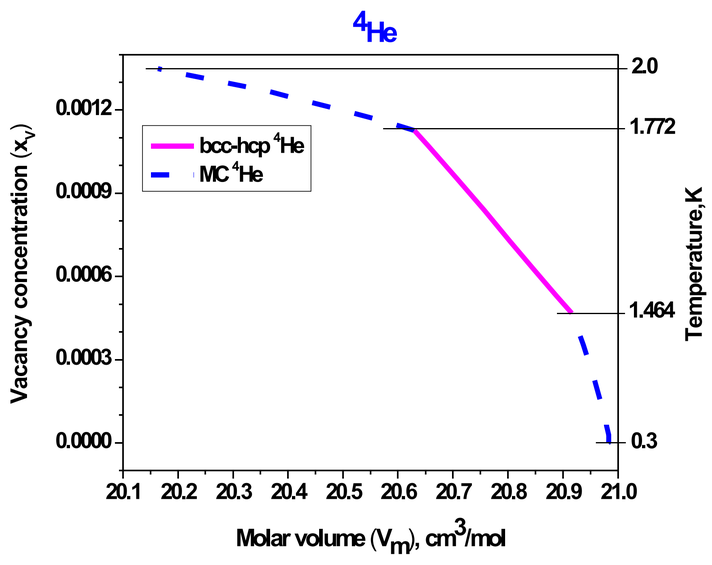
Hcp	Bcc
$Q_V = 5,92$ K	$Q_V = 4,19$ K
$\Theta_D = 26,30$ K	$\Theta_D = 26,89$ K
$x_V \sim 5 \cdot 10^{-4}$	$x_V \sim 4 \cdot 10^{-3}$

Results

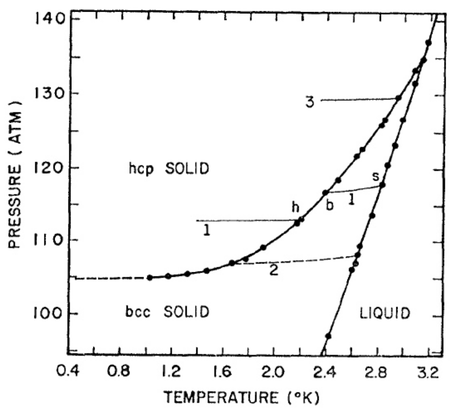
Phase diagram of ^{4}He



Vacancy concentration for hcp ^{4}He

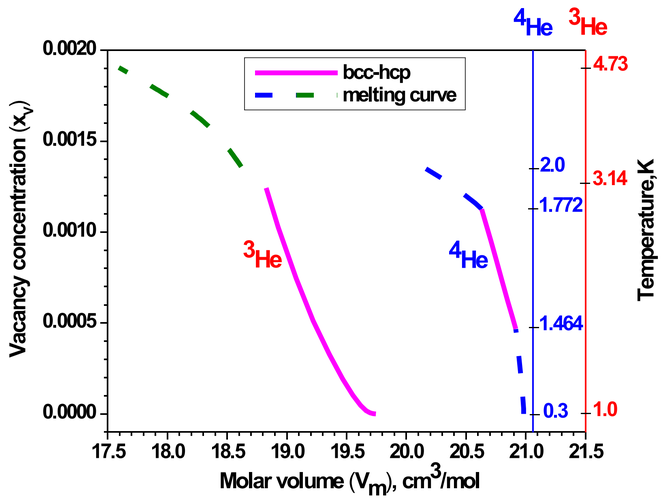


Phase diagram of ^{3}He



G. C. Straty and E. D. Adams, Phys. Rev. 150, 1, 123 (1966)

Vacancy concentration for both hcp ^{3}He and ^{4}He



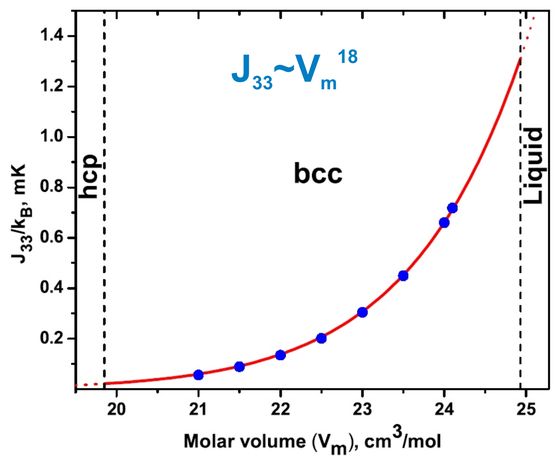
The same vacancy concentration on bcc-hcp region for both isotopes

Abstract

We analyze the problem of bcc phase existence in solid helium using identification of contributions of phonons and vacancies to thermodynamic properties. Phonons are considered within the classical Debye theory and vacancies are treated as wide-band quasi-particles according to Hetherington's approach [1]. The analysis of Debye temperature and vacancy activation energy, Q_V, was performed in wide molar volume range for hcp ^{4}He and bcc ^{3}He [2]. Using dependence $Q_V(V_m)$ [2], we estimate vacancy concentration, x_v, on the bcc-hcp pressure-temperature line for the both helium isotopes. It results in the same dependence of $x_v(V_m)$ for ^{3}He and ^{4}He under condition of V_m increasing by 10% in ^{4}He. It means that in high temperature range, where vacancy contribution is essential, the hcp lattice is destabilized by high value of x_v. We establish that wide-band vacancies destabilize the hcp lattice and tend it to the hcp-bcc phase transition under raising their concentration with temperature near the melting curve for both helium isotopes. The criterion for hcp phase destabilization is proposed.

[1] I.H. Hetherington, Phys. Rev. 176, 231 (1968)
[2] V.N. Grigorev and Ye.O. Vekhov, JLTP, 149, 41 (2007)

Exchange integral J_{33} *vs* molar volume of bcc ^{3}He as a quantum criterion of bcc phase existence



Data points - S. Trickey, W. Kirk, and E. Adams. Thermodynamic, elastic, and magnetic properties of solid helium. Rev. Mod. Phys., 44(4):668–715, 1972.

Thermodynamic estimations:

$$W_v = (x_v^{bcc} - x_v^{hcp})\, N_A\, k_B\, Q_V^{bcc}$$

W_V = 0.12 J/mol — the energy of extra vacancies are formatted under structural hcp-bcc transition

W_{PT} = 0.27 J/mol — phase transition latent heat

It means vacancy model proposed does not contradict to thermodynamics

Conclusions

	Vacancies	de Boer Parameter
No bcc phase	Ne, Ar, Kr, Xe: $\frac{Q_V}{T_m} \sim 20 - 25$	Xe – 0.009 Kr – 0.017 Ar – 0.033 Ne – 0.094
Bcc phase	^{4}He, ^{3}He: $\frac{Q_V}{T_m} \sim 3$ Large vacancy concentrations near T_m	^{4}He – 0.412 ^{3}He – 0.483 Huge zero-point vibrations

Acknowledgments

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