THE THERMAL CONDUCTION FROM THE CENTERS OF THE NUCLEAR REACTIONS IN SOLIDS

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If nuclear reactions happen in solids, heat generated from the reaction center is diffused. In this study, the thermal conduction from the centers of a DD reaction in solids induced by the Bose-Einstein condensation is considered. The voids in solids are assumed as the sites of the reaction centers. The equations of the thermal conduction are solved using Fourier expansion. The calculated results show the rapid temperature relaxation. This means that nuclear reactions in solids do not induce thermal explosions.

1 DD reaction rate in solid

In the previous work [1], DD reaction rate in Pd void is calculated applying the equivalent linear two-body (ELTB) method. The rate is determined by the ELTB ground state wave function $\Psi$ for $N$ identical charged Bose nuclei as

$$ R = -\frac{2\sum_{i<j} \langle \Psi | \text{Im} V_{ij}^F | \Psi \rangle}{\hbar \langle \Psi | \Psi \rangle}, \quad (1) $$

where imaginary part of Fermi pseudopotential $V_{ij}^F$ [2,3] is written as

$$ \text{Im} V_{ij}^F = -\frac{\mathcal{A} \hbar}{2} \delta(r_i - r_j). \quad (2) $$

The short-range interactions of nuclear forces between two Bose nuclei are introduced by using $\delta$ function. [2,3] The constant $A$ is given by the Bohr radius $r_B$ and the $S$ factor of the nuclear reaction between two nuclei as $A = 2S/\pi \hbar$. The ELTB solution also gives the critical temperature $T_c$ of Bose-Einstein condensation (BEC) by well known formula which is written as

$$ T_c = \frac{\hbar^2}{2\pi m k_B} \left( \frac{n}{\zeta(\frac{1}{2})} \right)^{2/3}, \quad (3) $$

where $n$ is the local number density of Bose particles and $\zeta(Z)$ is the Riemann’s zeta function. The probability of the ground-state occupation is given by

$$ \Omega = 1 - \left( \frac{T}{T_c} \right)^{2/3} \quad \text{for} \ T < T_c. \quad (4) $$

If the ground state occupation for $T < T_c$ is taken into account the fusion rate is given by $R_\Omega$. When $T \geq T_c$, no nuclear reactions happen because $\Omega = 0$. The trapped site for a deuteron cluster is shown in Figure 1. The calculated results for $T_c$ and $R$ are listed in
Table 1. When $N \geq 4$ with using non-linear screening [4,5], $T_c$ is higher than the room temperature. The ELTB solution is plotted in Figure 2 for the case of the 5 deuteron cluster trapped at VacO.

Table 1 The nuclear reaction rate $R [10^7 \text{sec}^{-1}]$ and the critical temperature $T_c [K]$ for the case of $N$ deuterons trapped at VacO in Pd.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Thomas-Fermi screening</th>
<th>non-linear screening</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>56 2.1</td>
<td>257 33.8</td>
</tr>
<tr>
<td>4</td>
<td>66 3.5</td>
<td>329 66.4</td>
</tr>
<tr>
<td>5</td>
<td>76 5.0</td>
<td>403 108.6</td>
</tr>
<tr>
<td>6</td>
<td>86 6.7</td>
<td>480 160.2</td>
</tr>
<tr>
<td>7</td>
<td>95 8.6</td>
<td>558 221.3</td>
</tr>
</tbody>
</table>

Figure 1. The structure of VacO in fcc lattice. The black and the gray circles mean occupied and unoccupied lattice points, respectively. These defects construct octahedral void, which is called VacO in this paper.

Figure 2. The ELTB solution for the system including 5 deuterons in VacO in fcc Pd. Non-linear screening potential is used as the DD interaction. The nondimensional quantity $x$ is defined as $x = \sqrt{\hbar/m_0} \rho$, where $\omega = 0.86 \times 10^{14} \text{sec}^{-1}$ and $\rho^2 = \Sigma r_i^2$. The solid line means the ELTB solution. The dashed lines mean each potential normalized by $|\epsilon| = 409$. ( $p/x^2$: component divided from the operators for kinetic energy, $qf/x$: screened DD repulsion potential, $\Sigma_{\text{col}}$: the lattice summation for the Coulomb potentials by host Pd ions. (see Ref.1) )
2 Thermal Conduction

If nuclear reactions happen in solids, heat generated from the reaction center is diffused. In this study, the thermal conduction from the center of a DD reaction in Pd is estimated. The equation of the thermal conduction in solid is written as

$$\frac{\partial T}{\partial t} = k \nabla^2 T,$$

(5)

where $T$ is the deviation of the temperature from the equivalent value and $t$ is the time from a reaction. The constant $k$ is defined as

$$k = K/C \rho,$$

(6)

where constants $K$, $C$ and $\rho$ mean the thermal conductivity ($75.5 \text{J/(sec m K)}$), the specific heat ($253 \text{(mol K)}$) and the density ($12.0 \text{g/cm}^3 = 12.0 \times 10^6 \text{g/cm}^3$), respectively. The initial condition used for solving Eq.(5) is $T = T_0$ in the $d \times d \times d$ cube and $T = 0$ for otherwise. In this condition, the parameter $d$ corresponds to the size of the deuteron cluster and the initial temperature is obtained by

$$T_0 = E/CM_0,$$

(7)

where constants $E$ and $M_0$ mean the energy generated from a DD reaction ($23.8 \text{MeV} = 23.8 \times 10^6 \times 1.60 \times 10^{-19} \text{J}$) and the number of moles in the $d \times d \times d$ cube ($4/\text{Avogadro number mol}$), respectively. The periodic boundary condition used for solving Eq.(5) is written as

$$X(x) = \begin{cases} 
0 & \text{for } 0 \leq x < \frac{L-d}{2} \\
T_0^{1/3} & \text{for } \frac{L-d}{2} \leq x \leq \frac{L+d}{2} \\
0 & \text{for } \frac{L+d}{2} < x \leq L
\end{cases},$$

(8)

and

$$X(x) = X(x+L).$$

(9)

A solution of Eq.(5) using Fourier expansion is written as

$$T = \sum_{n_x,n_y,n_z} C_{n_x} \cos(q_x x) e^{-kq_x^2} C_{n_y} \cos(q_y y) e^{-kq_y^2} C_{n_z} \cos(q_z z) e^{-kq_z^2},$$

(11)

where constants are defined as

$$q_i = \frac{2n_i \pi}{L} \quad \text{and} \quad C_{n_i} = (-1)^{n_i} \frac{2T_0^{1/3}}{n_i \pi} \sin \frac{n_i \pi d}{L}.$$

(12)

The parameter $L$ means distance between two neighboring reaction centers. This parameter is obtained by well known formula for the concentration of Shottky defect in solid. It is written as

$$n / N = e^{-w/k_BT},$$

(13)

where $n$, $N$ and $w$ mean the number of defect, the number of total atoms and vacancy formation energy ($\sim 1 \text{eV}$), respectively. Assuming the uniform distribution of the trapped sites, the parameter $L$ is obtained by
where \( a \) is the lattice constant of fcc Pd (3.89 Å). As the temperature is increased, the concentration of the vacancy is increased and the mean distance between vacancies is decreased. They are shown in Figures 3 and 5. The calculated result for the thermal conduction is plotted in Figure 5. The rapid relaxation can be seen in Figure 5.

\[
L = \frac{a}{4} \exp \left( \frac{\mu}{3k_bT} \right),
\]

(14)
Figure 6. The rise in temperature by the iterative DD reactions. In this case, the initial temperature is 300K. For the case of 5 deuteron cluster trapped at VacO, $T_c$ of BEC is 403K (see Table 1), which is shown by dashed line. After the $1.3 \times 10^8$ times iterative DD reactions, the temperature becomes higher than $T_c$ and BEC is broken.

3 Conclusions

1. If a DD reaction happens in a void, temperature of the reaction center becomes extremely high. However rapid recovery from the high temperature is seen, because thermal conductivities of metals are high. For the case of Figure 5, recovering time is smaller than $10^{10}$ sec. This is smaller than the inverse of the reaction rate $108.6 \times 10^7$ sec$^{-1}$. (see Table 1)

2. If iterative reactions happen, temperature raises slowly. This is shown in Figure 6. For the case of 5 deuteron cluster trapped at VacO, $T_c$ of BEC is 403K. (see Table 1) Seeing Figure 6, temperature becomes higher then $T_c$ after the $1.3 \times 10^8$ times iterative reactions. After that, local BEC in VacO is broken and DD reactions are stopped. This means that nuclear reactions in solid do not induce thermal explosions.

References