Brief Reports

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Relaxation times for nonlinear heat conduction in solid H_2

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The temperature distribution in solid crystalline hydrogen has been shown to be governed by the essentially nonlinear diffusion equation $\partial\Theta/\partial t = D\Theta^2\nabla^2\Theta$ in which there appears the dimensionless thermal variable $\Theta \equiv [1+(T/T_c)^4]^{-1}$ with the constants D and T_c dependent on the ortho-H_2 percentile. In the present communication, generic upper bounds are obtained on the cooling and warming relaxation times for a volume of solid H_2 subject to a constant-temperature-surface condition. Valid for H_2 solids of unrestricted size and shape, these generic upper bounds on the relaxation times apply for arbitrary initial-temperature distributions.

In solid crystalline molecular hydrogen, the temperature distribution $T = T(\vec{x}, t)$ is governed by the equation[1]

$$\frac{\partial\Theta}{\partial t} = D\Theta^2\nabla^2\Theta \tag{1}$$

in which the dimensionless thermal variable $\Theta = \Theta(\vec{x}, t) \equiv [1+(T/T_c)^4]^{-1}$ is patently positive but less than unity, and the diffusion constant appears as

$$D \equiv (415\ \text{cm}^2/\text{sec})/\chi T_c^3 = (1.69\ \text{cm}^2/\text{sec})/\chi(1+1.043\chi)^3\ , \tag{2}$$

with the ortho-H_2 fraction χ in the range $0.05 \lesssim \chi \lesssim 0.75$ and $T_c \equiv 6.26 + 6.53\chi$. Suppose that a volume $V = \int_R d^3x$ of solid H_2 occupies the spatial region R with the smooth bounding surface ∂R maintained at a constant temperature, so that $\Theta = \Theta_s$ ($\equiv$const) for all $\vec{x} \in \partial R$. Then the non-negative quantity

$$\Gamma = \Gamma(t) \equiv \int_R (\Theta^{-1} - \Theta_s^{-1})^2 d^3x \tag{3}$$

is a Liapunov functional,[2] since

$$\begin{aligned}\frac{d\Gamma}{dt} &= -2\int_R (\Theta^{-1}-\Theta_s^{-1})\Theta^{-2}\left(\frac{\partial\Theta}{\partial t}\right) d^3x \\ &= -2D\int_R (\Theta^{-1}-\Theta_s^{-1})\nabla^2\Theta\, d^3x \\ &= -2D\int_R \Theta^{-2}|\nabla\Theta|^2 d^3x \end{aligned}\tag{4}$$

by virtue of (1), Gauss's theorem, and $\Theta = \Theta_s$ over ∂R. Since the final member in (4) is patently negative definite, the Liapunov functional (3) decreases monotonically to zero with increasing t as Θ approaches Θ_s through the region. To obtain an upper bound on the relaxation time associated with the thermal adjustment $\Theta \to \Theta_s$, first observe that

$$\begin{aligned}\int_R \Theta^{-2}|\nabla\Theta|^2 d^3x &= \int_R \left|\nabla \ln\left(\frac{\Theta}{\Theta_s}\right)\right|^2 d^3x \\ &\geqq 3\left(\frac{\pi}{2}\right)^{4/3}\left(\int_R \left[\ln\left(\frac{\Theta}{\Theta_s}\right)\right]^6 d^3x\right)^{1/3} \\ &\geqq 3\left(\frac{\pi}{2}\right)^{4/3} V^{-2/3}\int_R \left[\ln\left(\frac{\Theta}{\Theta_s}\right)\right]^2 d^3x\ , \end{aligned}\tag{5}$$

where use is made of a Sobolev inequality[3] for the third member and a Hölder inequality for the final member.[4] By combining (5) with (4), one obtains

$$\frac{d\Gamma}{dt} \leqq -6\left(\frac{\pi}{2}\right)^{4/3} V^{-2/3} D\int_R \left[\ln\left(\frac{\Theta}{\Theta_s}\right)\right]^2 d^3x\ . \tag{6}$$

The two cases of practical importance are treated separately:

Cooling: $\Theta \leqq \Theta_s$. Define $\hat{\Theta} \equiv \min_{\vec{x}\in R}\Theta(\vec{x}, 0)$, corresponding to the maximum initial temperature in the solid; then with $\hat{\Theta} \leqq \Theta \leqq \Theta_s$ it follows that

$$\ln\left(\frac{\Theta_s}{\Theta}\right) \geqq \left[(\hat{\Theta}^{-1}-\Theta_s^{-1})^{-1}\ln\left(\frac{\Theta_s}{\hat{\Theta}}\right)\right](\Theta^{-1}-\Theta_s^{-1}) \tag{7}$$

from the convexity (i.e., negative second derivative) of the logarithm. By applying (7) to (6), one obtains

$$\frac{d\Gamma}{dt} \leqq -\tau_c^{-1}\Gamma\ , \tag{8}$$

where

$$\tau_c = (0.0913)V^{2/3}D^{-1}(\hat{\Theta}^{-1}-\Theta_s^{-1})^2\left[\ln\left(\frac{\Theta_s}{\hat{\Theta}}\right)\right]^{-2}. \tag{9}$$

The solution to the differential inequality (8),

$$\Gamma(t) \leqq \Gamma(0) e^{-t/\tau_c}, \tag{10}$$

shows that the Liapunov functional (3) approaches zero with a characteristic relaxation time less than or equal to the quantity (9). Hence, (9) is a rigorous upper bound on the relaxation time for cooling.

Warming: $\Theta \geqq \Theta_s$. In this case the lower bound on the logarithm

$$\ln(\Theta/\Theta_s) \geqq 1 - \Theta_s \Theta^{-1} \tag{11}$$

in combination with (6) yields

$$\frac{d\Gamma}{dt} \leqq -\tau_w^{-1}\Gamma, \tag{12}$$

where

$$\tau_w = (0.0913) V^{2/3} D^{-1} \Theta_s^{-2}. \tag{13}$$

In view of (12), the Liapunov functional (3) approaches zero with a characteristic relaxation time less than or equal to (13), and thus the latter quantity is a rigorous upper bound on the relaxation time for warming.

It is of interest to evaluate (9) and (13) for parameter values pertinent to current experiments[5] on solid hydrogen in the sample chamber of a dilution refrigerator: $V = 0.10$ cm^3, $\chi = 0.125$, $D = 9.36$ cm^2/sec [according to (2)], $T_c = 7.08$, $\Theta_s = 1.000$ for cooling with, for example, $\hat{\Theta} = 0.890$ (corresponding to a maximum temperature in the solid of 4.20 K) and $\Theta_s = 0.890$ for warming; these parameter values yield $\tau_c = 2.36$ msec and $\tau_w = 2.65$ msec.

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[1]G. Rosen, Phys. Rev. B 19, 2398 (1979).

[2]See, for example, W. Hahn, *Theory and Application of Liapunov's Direct Method* (Prentice-Hall, Englewood Cliffs, 1963), pp. 132–139. Distinct Liapunov functionals have recently been considered for a class of related nonlinear diffusion equations by J. G. Berryman, J. Math. Phys. 21, 1326 (1980).

[3]G. Talenti, Ann. Pura Appl. 110, 353 (1976); G. Rosen, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. 21, 30 (1971); E. H. Lieb, Rev. Mod. Phys. 48, 553 (1976). For ϕ continuous and with piecewise-continuous first derivatives through unbounded Euclidean space, the Sobolev inequality $\int |\nabla\phi|^2 d^3x \geqq 3(\pi/2)^{4/3}(\int \phi^6 d^3x)^{1/3}$ holds if the integral on the right side is finite. This inequality, involving integrals over unbounded Euclidean space, is adapted in (5) by putting $\phi = \ln(\Theta/\Theta_s)$ for $\vec{x} \in R$ and $\phi \equiv 0$ for $\vec{x} \notin R$.

[4]In the event that the shape of R admits solution to the Helmholtz eigenvalue problem $\nabla^2\psi = -\lambda^2\psi$ for $\vec{x} \in R$, $\psi = 0$ for $\vec{x} \in \partial R$, then (5) can be sharpened by using the smallest eigenvalue $\lambda^2_{\min}$ in place of $3(\pi/2)^{4/3} V^{-2/3}$ ($< \lambda^2_{\min}$) and omitting the third member that appears in (5). Such a specialized calculation would result in a smaller numerical coefficient and the appearance of dimensionless shape factors in (9) and (13).

[5]See, for example, G. Rosen and R. W. H. Webeler, Lett. Nuovo Cimento 26, 579 (1979).