ON HEAT TRANSFER IN ULTRA-PURE MATERIALS

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Summary Unsteady heat transfer in ultra-pure materials is discussed in the lecture. Closed equations for the heat propagation for sample systems are obtained and their analytical solutions are constructed. The results are confirmed by computer simulations.

INTRODUCTION

Thermomechanical processes in ultra-pure materials differ substantially from the processes observed in a usual material. In particular, Fourier's law of heat conduction is not fulfilled in low dimensional ultra-pure materials. This is confirmed by analytical [1, 2, 3] and experimental [4, 5, 6] investigations. The covariance analysis [7, 8] allows to solve analytically the heat conduction problems for harmonic models of such materials, which are relevant to low-dimensional nanostructures. In the lecture closed equations for the heat propagation for sample systems are obtained and their analytical solutions are constructed. Deviations from the classical thermal transfer processes are analysed.

THE SAMPLE MODEL

Let us consider an example of infinite one-dimensional crystal (a chain of interacting particles). The dynamics equation we write in the form

$$\dot{u} = v\,, \qquad \dot{v} = \mathcal{L}u + b\dot{W}, \tag{1}$$

where $u,\ v,\ b$ are scalar functions of time and spatial discrete variable n; $\mathcal{L}$ is a linear difference operator of 2-th order, W is Wiener stochastic process; the dot indicates the time derivative. The quantities u and v describe particle displacement and velocity, b is the intensity of the random external action on the system. The simplest variant of operator $\mathcal{L}$ is

$$\mathcal{L}u(n) = \omega_0^2 \Big(u(n+1) - 2u(n) + u(n-1)\Big)\,, \tag{2}$$

where $\omega_0 \stackrel{\text{def}}{=} \sqrt{C/m}$ is the frequency of the basic oscillator, m is the the particle mass, C is the bond stiffness. More complex operators can take into account the interaction between distant particles, elastic support and etc. The initial conditions are

$$u|_{t=0} = \sigma_u \rho_u\,, \qquad v|_{t=0} = \sigma_v \rho_v, \tag{3}$$

where ρ_u and ρ_v are random functions of n with zero expectation and unit variance, σ_u and σ_v are deterministic functions of n.

DYNAMICS OF COVARIANCES

Let us introduce covariance variables

$$\xi(p,q) \stackrel{\text{def}}{=} \big\langle u(p)u(q)\big\rangle\,, \qquad \kappa(p,q) \stackrel{\text{def}}{=} \big\langle v(p)v(q)\big\rangle\,, \qquad \nu_1(p,q) \stackrel{\text{def}}{=} \big\langle v(p)u(q)\big\rangle\,, \qquad \nu_2(p,q) \stackrel{\text{def}}{=} \big\langle u(p)v(q)\big\rangle\,, \tag{4}$$

where angular brackets stand for mathematical expectation. Differentiation of these variables using equations of motion (1) gives a closed system of differential equations for covariances:

$$\begin{aligned} &\dot{\xi} = \nu_1 + \nu_2\,, && \dot{\nu}_1 = \kappa + \mathcal{L}_p\xi, \\ &\dot{\kappa} = \mathcal{L}_q\nu_1 + \mathcal{L}_p\nu_2 + \beta\,, && \dot{\nu}_2 = \kappa + \mathcal{L}_q\xi, \end{aligned} \tag{5}$$

where $\beta(p,q) \stackrel{\text{def}}{=} b(p)b(q)\delta_{pq}$; $\delta_{pq} = 1$ for $p = q$ and it is zero otherwise. This system can be reduced to closed systems of two equations of the second order

$$\left\{\begin{aligned} &\ddot{\xi} = 2\kappa + (\mathcal{L}_p + \mathcal{L}_q)\xi, \\ &\ddot{\kappa} = (\mathcal{L}_p + \mathcal{L}_q)\kappa + 2\mathcal{L}_p\mathcal{L}_q\xi + \dot{\beta}; \end{aligned}\right. \qquad \left\{\begin{aligned} &\ddot{\nu}_1 = (\mathcal{L}_p + \mathcal{L}_q)\nu_1 + 2\mathcal{L}_p\nu_2 + \beta, \\ &\ddot{\nu}_2 = 2\mathcal{L}_q\nu_1 + (\mathcal{L}_p + \mathcal{L}_q)\nu_2 + \beta \end{aligned}\right. \tag{6}$$

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or to one equation of the 4-th order

$$\dddot{\xi} - 2(\mathcal{L}_p + \mathcal{L}_q)\ddot{\xi} + (\mathcal{L}_p - \mathcal{L}_q)^2\xi = 2\dot{\beta}. \tag{7}$$

The similar equations of the 4-th order can be obtained for variables κ, $\dot{\nu}_1$, $\dot{\nu}_2$, where the difference will be only in the right parts of the equations, which are, respectively,

$$\left(\tfrac{\partial}{\partial t} - \mathcal{L}_p - \mathcal{L}_q\right)\dot{\beta}\,, \qquad \left(\tfrac{\partial}{\partial t} + \mathcal{L}_p - \mathcal{L}_q\right)\dot{\beta}\,, \qquad \left(\tfrac{\partial}{\partial t} - \mathcal{L}_p + \mathcal{L}_q\right)\dot{\beta}. \tag{8}$$

CONTINUALIZATION

Let us change from discrete spatial variables p, q to variables

$$x \stackrel{\text{def}}{=} a\,\tfrac{p+q}{2}\,, \qquad n \stackrel{\text{def}}{=} q - p, \tag{9}$$

where x is continuum spatial variable, n is discrete correlational variable, and a is the lattice constant. If the processes are relatively slow in time, and the spatial functions are relatively smooth in space, then for the case (2) the equation (7) can be reduced to

$$\ddot{\theta}_n + \tfrac{1}{4}c^2(\theta_{n+1} - 2\theta_n + \theta_{n-1})'' = \dot{\chi}\delta_n, \tag{10}$$

where $\delta_n = \delta_{pq}$, prime stands for x-derivative, c is the sound speed, θ_n is the nonlocal temperature [9], and χ is the heat supply intensity defined as

$$c \stackrel{\text{def}}{=} a\omega_0\,, \qquad \theta_n(x) \stackrel{\text{def}}{=} (-1)^n\,\frac{m}{k_B}\left\langle v(p)\,v(q)\right\rangle\,, \qquad \chi \stackrel{\text{def}}{=} \frac{m}{2k_B}\,b^2, \tag{11}$$

where k_B is the Boltzmann constant. The initial conditions for equation (10) are

$$\theta_n|_{t=0} = T_0(x)\delta_n\,, \qquad \dot{\theta}_n|_{t=0} = 0, \tag{12}$$

where $T_0(x) = \frac{1}{2k_B}m\sigma_v^2(x)$ is the initial temperature distribution, σ_u is accepted to be zero. The initial conditions (7) are taken after a fast transition process, which results, according to the virial theorem, in a double reduction of the initial kinetic temperature [10]. Note that in contrast with the random initial value problem (1), (3) the initial value problem (10), (12) is expressed in terms of mathematical expectations, and therefore it is a deterministic problem.

Analytical solution of problem (10), (12) yields

$$T(t,x) = \frac{1}{\pi}\int_{-ct}^{ct}\frac{T_0(x-y)}{\sqrt{c^2t^2-y^2}}\,dy + \frac{1}{\pi c}\int_0^t\int_{-c\tau}^{c\tau}\ln\left(\frac{c\tau+\sqrt{c^2\tau^2-y^2}}{|y|}\right)\dot{\chi}(t-\tau,x-y)\,dy\,d\tau. \tag{13}$$

where $T(x) \equiv \theta_0(x)$ is the kinetic temperature. Thus we have integral representation of the temperature profile in the crystal. In the lecture explicit solutions for selected variants of $T_0(x)$ and $\chi(x,t)$ are obtained and compared with numeric solutions. Several additional problems of heat conduction in ultra-pure materials are presented and discussed in the lecture.

CONCLUSIONS

Unsteady heat conduction problems for ultra-pure materials can be solved effectively using covariance analysis. The resulting solutions differs substantially from solutions obtained on the basis of classical heat conduction. The obtained results can be used to predict heat transfer properties of low-dimensional nanostructures.

References

[1] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet: Fourier's law: a challenge to theorists, in *Mathematical Physics 2000*, edited by A. Fokas *et al.* (Imperial College Press, London, 2000), p. 128–150.

[2] S. Lepri, R. Livi, and A. Politi: Thermal conduction in classical low-dimensional lattices, Phys. Rep. **377**, 1–80, 2003.

[3] A. Dhar: Heat transport in low-dimensional systems, Advances in Phys. **57**, 457–537, 2008.

[4] C. W. Chang, D. Okawa, H. Garcia, A. Majumdar, and A. Zettl: Breakdown of fourier's law in nanotube thermal conductors, Phys. Rev. Lett. **101**, 075903, 2008.

[5] X. Xu, L. F. Pereira, Y. Wang, J. Wu, K. Zhang, X. Zhao, S. Bae, C. T. Bui, R. Xie, J. T. Thong, B. H. Hong, K. P. Loh, D. Donadio, B. Li, and B. Ozyilmaz: Length-dependent thermal conductivity in suspended single-layer graphene, Nature Communications **5**, 3689, 2014.

[6] T. K. Hsiao, B. W. Huang, H. K. Chang, S. C. Liou, M. W. Chu, S. C. Lee, and C. W. Chang: Micron-scale ballistic thermal conduction and suppressed thermal conductivity in heterogeneously interfaced nanowires, Phys. Rev. B **91**, 035406, 2015.

[7] Z. Rieder, J. L. Lebowitz, and E. Lieb: Properties of a harmonic crystal in a stationary nonequilibrium state, J. Math. Phys. **8**, 1073–1078, 1967.

[8] A. M. Krivtsov: Heat transfer in infinite harmonic one-dimensional crystals. Doklady Physics 60, 407–411, 2015.

[9] A. M. Krivtsov: On unsteady heat conduction in a harmonic crystal. ArXiv:1509.02506, 2015.

[10] A. M. Krivtsov: Energy oscillations in a one-dimensional crystal. Doklady Physics **59**, 427–430, 2014.