Supplementary Material for

Mechanistic Transition of Heat Conduction in Two-Dimensional Solids: A Study of Silica Bilayers

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I. SUPPLEMENTARY FIGURES AND FIGURE CAPTIONS

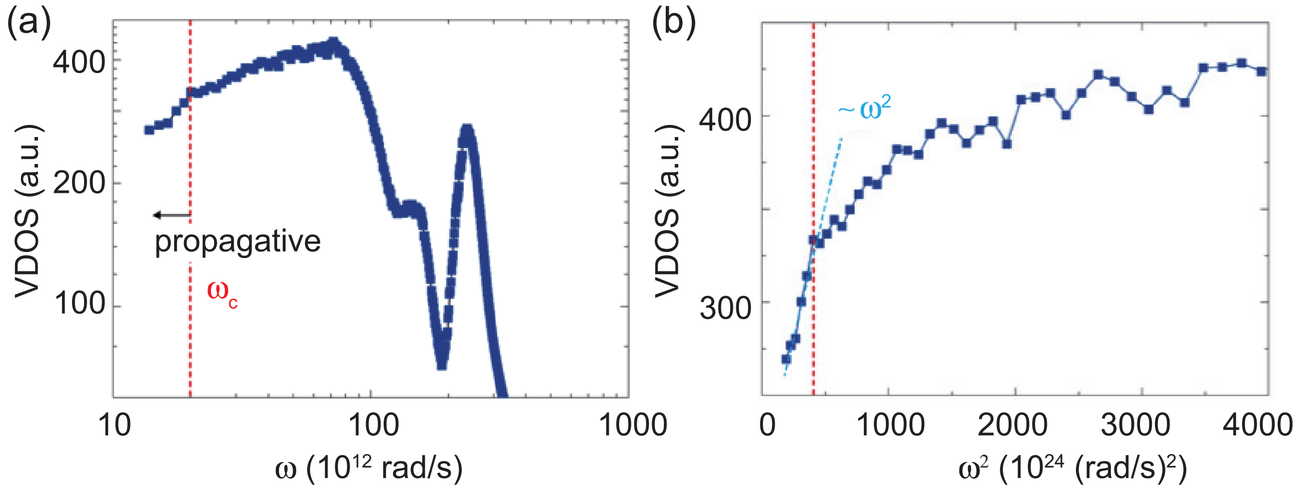

FIG. 1. (color online) (a-b) VDOS of 2D silica with $\alpha = 0.5$. The red dash line denotes a frequency cutoff $\omega_c = 20.10 \times 10^{12}$ rad/s below which vibrational modes are considered as propagating in the AF model, which follows the Debye model $\mathrm{DOS}\,(\omega) = 3V\omega^2/2\pi^2 v_s^3$.

II. THE DEFINITION OF LOCALIZATION FACTOR

The localization factor (LF) of spatial heat flux distribution is derived from the structural entropy $S_{\rm str}$ and the spatial filling factor q[1]. From our NEMD simulations, the intensity of heat flux distribution J_i ($i = 1, \ldots, N$) can be measured at a specific coarsening level, which is normalized first. Then the filling factor q is defined as

$$q = \frac{D}{N}, D = \frac{1}{\sum_{i=1,N} J_i^2} \tag{1}$$

The Shannon and Rényi entropies of the distribution are

$$S_1 = \sum_{i=1,N} J_i \log J_i, S_n = \frac{1}{1-n} \log(\sum_{i=1,N} J_i^n), \tag{2}$$

The difference between S_1 and S_2 characterize the structure of distribution and $S_{\rm str}$ can be defined as

$$S_{\rm str} = S_1 - S_2 = S_1 - \log D \tag{3}$$

In order to obtain the localization factor of a spatial distribution, an error function is calculated

$$E(\varepsilon) = [S_{\rm str}(q)_{\rm MD} - S_{\rm str}(q)_{\exp(-x^\varepsilon)}]^2 \tag{4}$$

The exponent ε is the localization factor, where the extremes $\varepsilon = 0$ and $\propto$ correspond to totally flat and vertical-walled features, respectively.

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[1] A. Bonyár, L. M. Molnár, and G. Harsányi, Micron **43**, 305 (2012).