Ecole Centrale Paris, France

ANOMALOUS THERMAL CONDUCTIVITY OF AMORPHOUS NANO-SIZED THIN FILMS AND TUBES DUE TO SURFACE PHONON-POLARITONS

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Surface Phonon Polaritons (SPP)

⇒ SPP are evanescent electromagnetic waves that propagate along the interface of polar dielectrics, such as SiC and SiO_2.

⇒ They are generated by the coupling between the photons of the electromagnetic waves and the optical phonons of the materials.

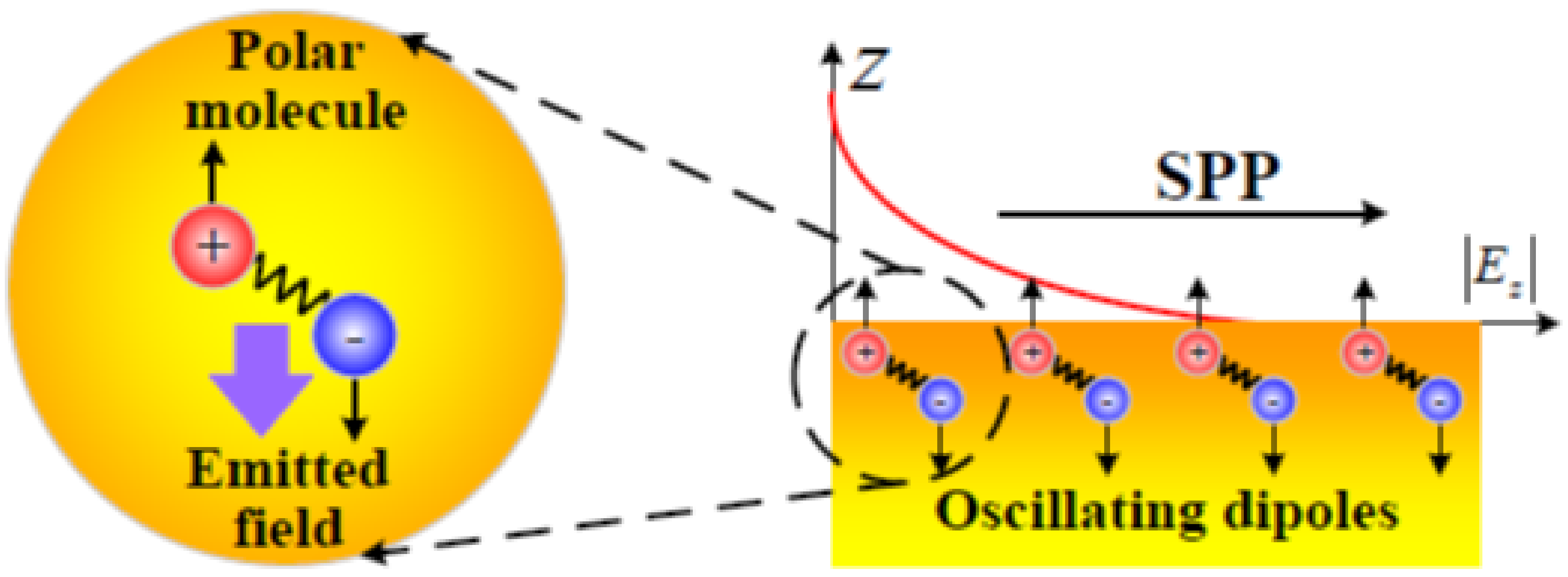

Fig. 1 Schematics of the generation and propagation of SPP.

⇒ These surface waves can be applied to improve the thermal performance of nanoscale devices in electronics **[1]**.

⇒ In this work, the thermal conductivity due to the propagation of SPP along a nano thin film and nanotube of SiO_2 is determined analytically.

Thermal Conductivity Model

⇒ The thin film, tube and their surrounding media are assumed to be **nonmagnetic** (**$\mu_0 = 1$**).

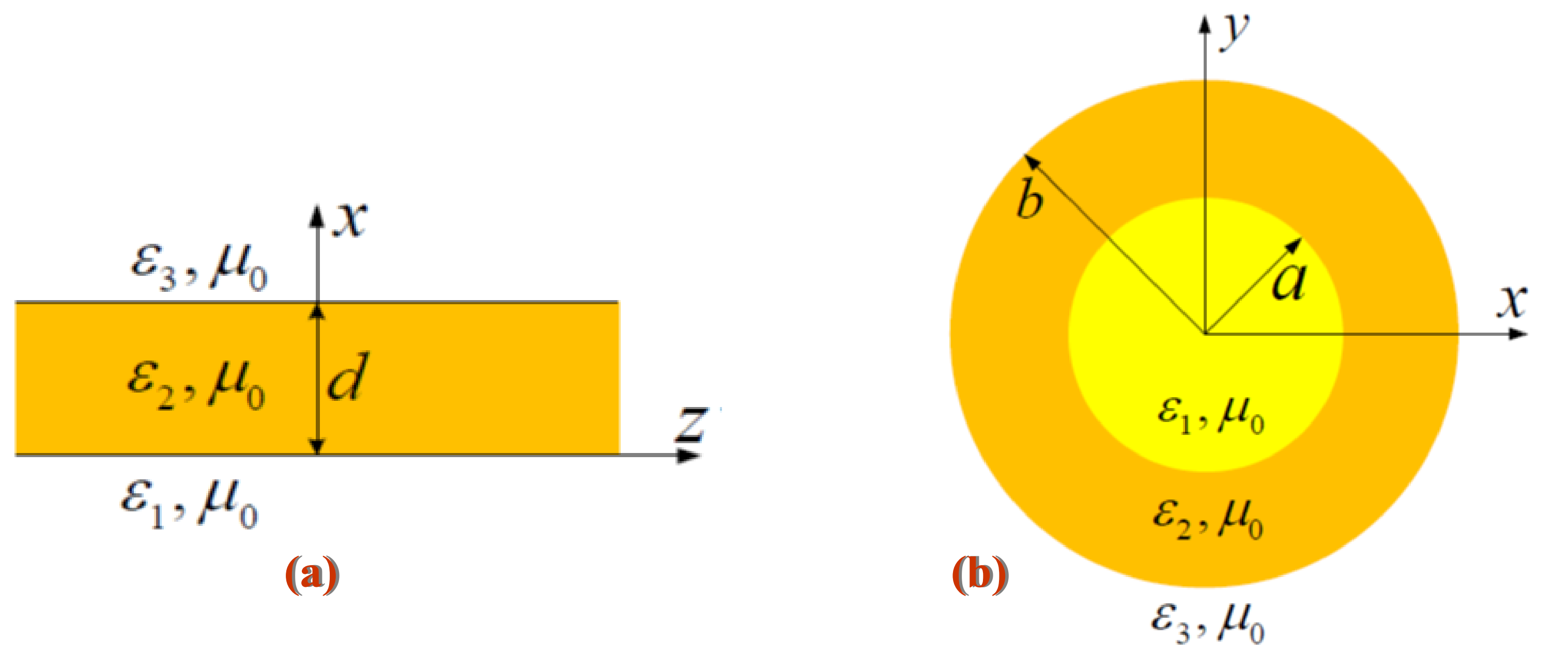

Fig. 2 Cross section of the **(a)** nano thin film and **(b)** nanotube under consideration.

⇒ The permittivities of the substrate (KBr) and superstrate (air) are **$\varepsilon_1 = 1.24$** and **$\varepsilon_3 = 1$**, respectively.

⇒ The permittivity ε_2 of the thin film or tube of SiO_2 change with the excitation frequency and is shown in Fig. 3.

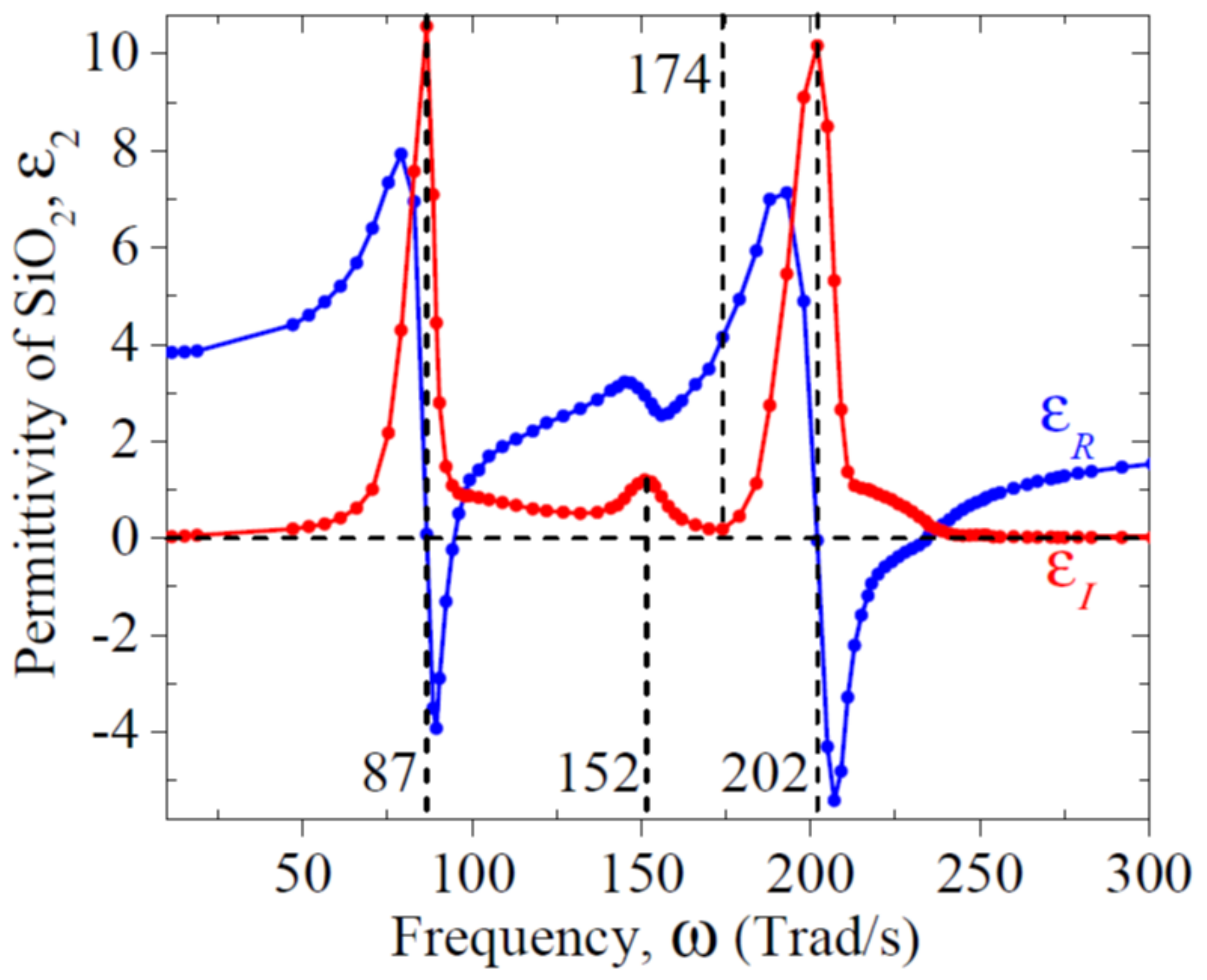

Fig. 3 Real and imaginary parts of the permittivity $\varepsilon_2 = \varepsilon_R - i\varepsilon_I$ of SiO_2 as a function of frequency **[2]**.

⇒ Based on the **Boltzmann transport equation** and **Maxwell equations**, the SPP thermal conductivity is given by

Nano thin film

$$\kappa = \frac{1}{4\pi d}\int_0^\infty \hbar\omega\Lambda\beta_R \frac{\partial f_0}{\partial T}\, d\omega$$

$$\boxed{\beta = \beta_R - i\beta_I}$$

In-plane wave vector (*z* axis in **Fig. 2**)

$$\boxed{\beta_I = C(\omega)\left[1-\left(\frac{d_c}{d}\right)^4\right]} \quad \boxed{d_c = \frac{\sqrt{\Delta}}{\varepsilon_3 k_0}\frac{|\varepsilon_2|}{|\varepsilon_2-\varepsilon_1|}}$$

$$\Delta = \varepsilon_1 - \varepsilon_3$$

Critical thickness

Nanotube

$$\kappa = \frac{1}{6\pi^2}\int_0^\infty \hbar\omega\Lambda\beta_R^2 \frac{\partial f_0}{\partial T}\, d\omega$$

$$\boxed{\Lambda = \frac{1}{2\beta_I}}$$

Propagation length of SPP

$$\boxed{\beta = k_0\sqrt{\frac{2\varepsilon_1\varepsilon_2}{(1-\rho)\varepsilon_1 + (1+\rho)\varepsilon_2}}}$$

$$\rho = (a/b)^n \quad n = 1,2,3,\ldots \quad k_0 = \omega/c$$

Azimuthal modes

$d \to d_c \Rightarrow \Lambda \to \infty$ ⇒ **Giant propagation length** ⇒ **High SPP thermal conductivity**

Propagation lengths

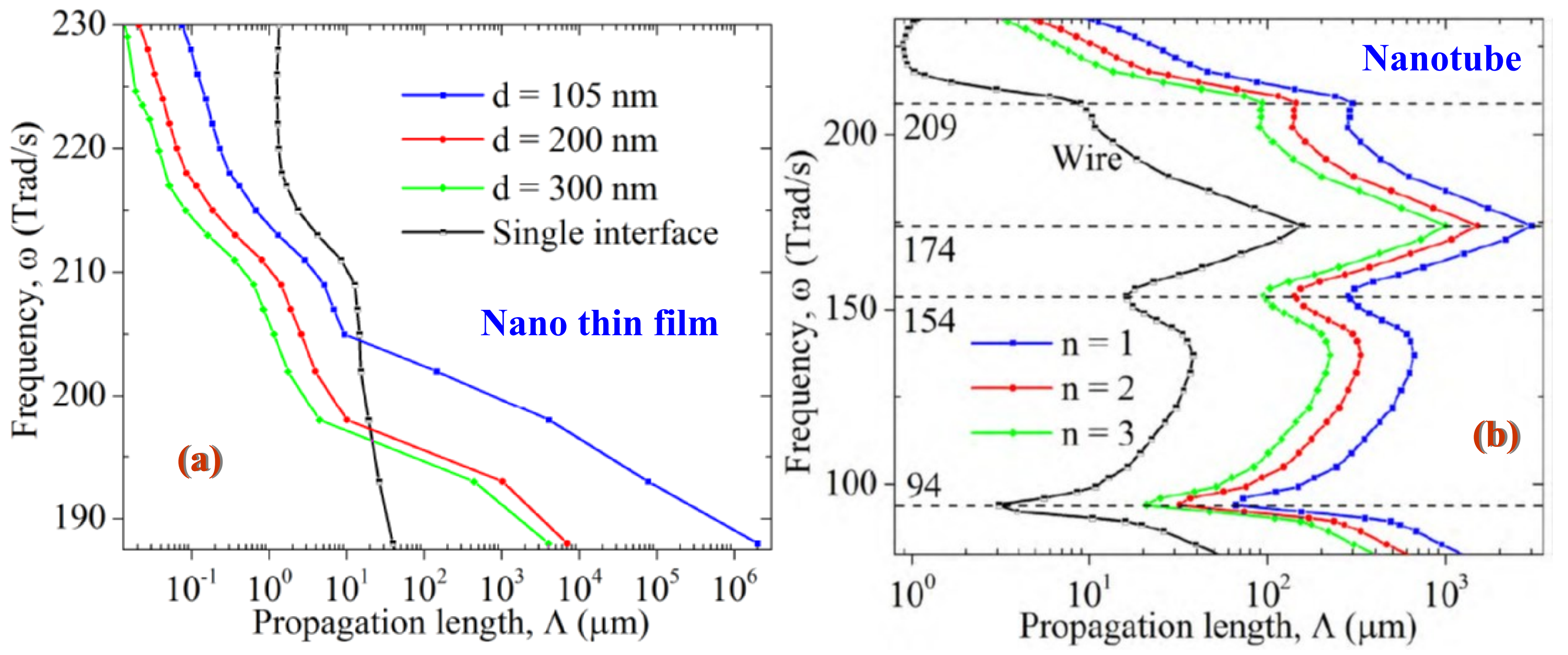

Fig. 4 Propagation length for a **(a)** nano thin film and **(b)** nanotube of SiO_2 as a function of frequency.

⇒The propagationof surface phonon-polaritons is present in a broad band of frequencies.

⇒The propagation length is larger at the frequency where the absorption of energy is minimal.

⇒The thinner the film or tube, the larger the propagation length.

⇒The first azimuthal mode (**n = 1**) exhibits the largest propagation length.

Poynting Vector Energy Flux

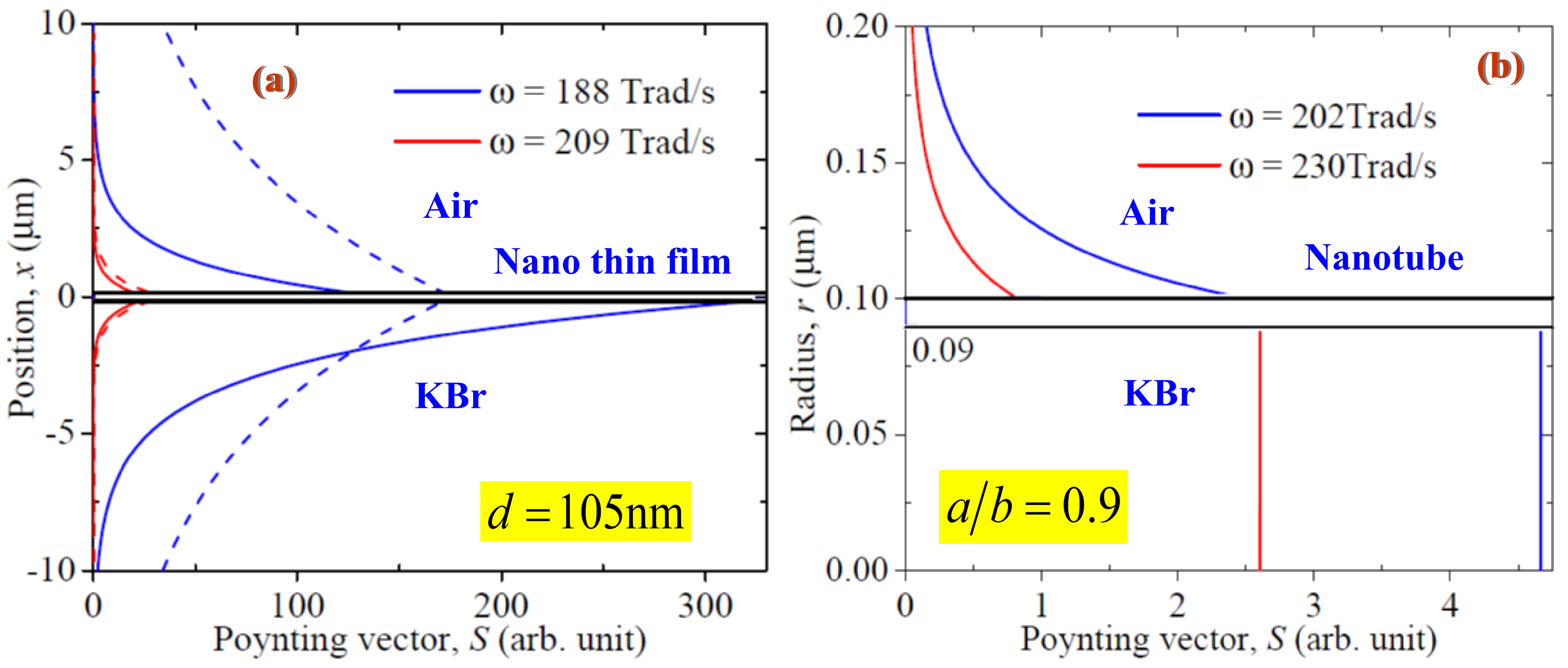

Fig. 5 Poynting vector energy flux for a **(a)** nano thin film and **(b)** nanotube of SiO_2.

⇒ The energy flux is negligible inside the film or tube, and it propagates along the interfaces with the surrounding media, mainly. **THERE ARE SPP!**

⇒ The absorbtion of energy depends on the frequency and it is higher in KBr than in air.

⇒ The propagation length increases with the Poynting vector energy flux.

Thermal Conductivity

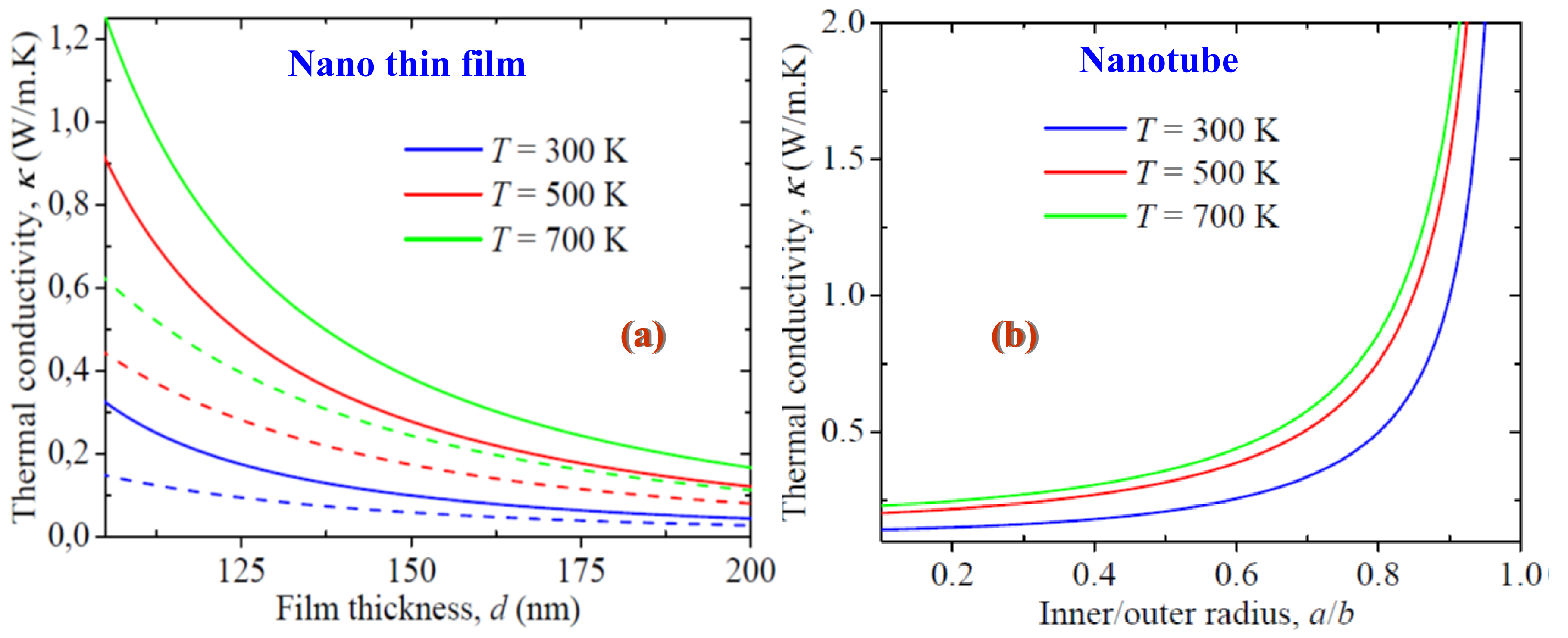

Fig. 6 SPP thermal conductivity of a **(a)** nano thin film and **(b)** nanotube of SiO_2.

⇒ The SPP thermal conductivity of the film or tube increases as their thickness decreases.

⇒ The SPP thermal conductivity increases with the temperature.

⇒ The SPP thermal conductivity of both the film and tube of SiO_2 can be as high as the bulk phonon counterpart (1.4 W/m.K).

⇒ A higher SPP thermal conductivity is obtained for the asymetric system (**$\varepsilon_1 \neq \varepsilon_3$**) than that for the symmetric one (**$\varepsilon_1 = \varepsilon_3$**).

⇒ This increase is about 100% for a 125 nm-thick thin film at room temperature.

Conclusions

1. The thermal conductivity due to surface phonon-polaritons increases when the material size reduces and the temperature increases.
2. The SPP thermal conductivity is significant at nanoscales and becomes negligible at microscales.
3. The propagation of SPP can be analyzed under a fully analytical approach for nano thin films and nanotubes.
4. A small difference on the permittivities of the surrounding media of a nano thin film can generate large propagation lengths and therefore high SPP thermal conductivities.

The propagation of surface phonon-polaritons has the potential to offset the reduction of the phonon thermal conductivity of polar dielectrics as their size is scaled down.

[1] J. Ordonez-Miranda et al., J. Appl. Phys. 113, 084311 (2013).
[2] E. D. Palik, *Handbook of optical constants of solids* (Academic press, Orlando, 1997).