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# Comment on “Simultaneous density and thermal conductivity depth profile reconstructions from noised thermal-wave amplitude and phase data using a combined integral equation and imperialist competitive algorithm method” [J. Appl. Phys. 133, 055102 (2023)]

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In a recent paper, Mandelis et al. [J. Appl. Phys. 133, 055102 (2023)] describe a photothermal methodology and a new inversion technique which, when applied to a heterogeneous material, is claimed to allow a *simultaneous reconstruction* of the depth profiles of thermal conductivity and density (assuming that the specific heat is a known constant). In this Comment we recall that, for the thermophysical configuration considered, the thermal conductivity and volumetric heat capacity (VHC) profiles cannot be identified simultaneously because they are fully correlated. The exposed problem exhibits unconditional non-identifiability leading to the non-uniqueness of the solution. The apparent success of the inversion tests does not preclude the fact that, for any (apparently) optimal solution, an infinite multiplicity of equally satisfactory pairs of conjugate profiles can be built. The simultaneous identification of the density and thermal conductivity profiles is here an unsolvable inverse problem.

## I. INTRODUCTION

In a recent paper,<sup>1</sup> Mandelis and coworkers present an inversion technique based on a new thermal-wave direct model coupled with a method of global optimization. This methodology is intended for photothermal depth profiling of heterogeneous materials, which consists in applying a periodic heat flux to the surface of a material and analyzing the temperature response of this same surface (through amplitude and phase frequency scans), in order to identify depth profiles of one or more thermal properties (the analysis in Ref. 1 considers one-dimensional heat transfer in a thermally thick material, which allows to consider a semi-infinite model). The thermal properties appearing as variable coefficients in the heat equation and the boundary condition are the thermal conductivity  $k(x)$  ( $x$  is the depth coordinate) and the volumetric heat capacity (VHC)  $C(x) \equiv \rho(x)c(x)$  (where  $\rho$  is the density and  $c$  the specific heat). From these profiles, those of diffusivity and effusivity are defined respectively as  $a(x) \equiv k(x)/C(x)$  and  $b(x) \equiv \sqrt{k(x)C(x)}$ . In fact, two of these four profiles allow us to deduce the other two. There is an abundant literature on photothermal depth profiling, considering both modulated and pulsed thermal stimuli. A consistent approach is to extract from the temperature data one among the four profiles mentioned above, provided that another is known independently; most often, VHC if assumed to be a known scalar. In Ref. 1, it is claimed that with the thermophysical configuration described above, it is possible, using the new inversion tool, to simultaneously reconstruct  $k(x)$  and  $\rho(x)$  (which amounts to say  $k(x)$  and  $C(x)$ , since the specific heat was taken as constant and known), without any *a priori* information. In this Comment we show, based on work on modeling heat transfer in graded heterogeneous media<sup>2,3</sup>, that the thermal conductivity and VHC profiles (in short  $k$ - $C$  profiles) are fully correlated when considering surface temperature. Attempting to identify them simultaneously is therefore hopeless, since there are infinitely many combinations of  $k$ - $C$  profiles leading to the same

surface-temperature dynamics. We will elaborate on the basic reasons for this non-identifiability. We will also discuss a trap known as inverse crime<sup>4</sup> which is known to produce overly optimistic inversion results.

## II. THERMAL MODEL AND LIOUVILLE TRANSFORMATION

In the Fourier space, the heat equation and the boundary condition for the problem considered in Ref. 1, express as:

$$C(x)pT = \frac{d}{dx} \left( k(x) \frac{dT}{dx} \right); \quad 0 \leq x < +\infty, \quad (1a)$$

$$P = -k(x) \frac{dT}{dx}; \quad x = 0, \quad (1b)$$

where  $p = i\omega$  is the Fourier variable,  $\omega$  is the modulation angular frequency,  $T$  and  $P$  are the temperature and the prescribed flux, respectively. The expressions in Eqs. (1a) and (1b) also represent the transient case, when considering  $T$  and  $P$  as the Laplace transforms of the temperature and surface flux, respectively, and  $p$  as the Laplace variable. Everything that will be said subsequently concerns the periodic regime and the transient regime indiscriminately.

The conductivity profile and the VHC profile appear in different terms in Eq. (1a). Could it be that their influences on the temperature data are different enough to allow simultaneous identification? No sensitivity analysis has been presented in Ref. 1 that would prove this.

Before looking at heterogeneous materials, let us recall that, for homogeneous materials, the surface temperature takes the simple expression:  $T = P/(b\sqrt{p})$ . Conductivity and VHC have merged to show only the effusivity  $b$ , which is therefore the only parameter accessible by inversion of the temperature data. It is not possible to evaluate conductivity and VHC separately. Exposed to non-identifiability in the case of uniform

properties, we might fear that the same is true in the presence of heterogeneous materials. This fear will be confirmed next by delving into the Liouville space.

The Liouville transformation allows to change a Sturm-Liouville differential equation into an equation in so-called Liouville normal form<sup>5,6</sup>. For the purposes of this discussion we will restrict ourselves to the first part of the transformation, which consists in changing the independent variable  $x$  into  $\xi$ :

$$\xi(x) \equiv \int_0^x \sqrt{C(x')/k(x')} dx'. \quad (2)$$

$\xi(x)$ , whose unit is  $s^{-1/2}$ , can be interpreted as the Square Root of the Diffusion Time (SRDT) from the surface to depth  $x$ , taking into account the diffusivity variations along this path.  $\xi(x)$  is a monotonically increasing function, which implies a one-to-one mapping between  $x$  and  $\xi$ . Going from  $x$  to  $\xi$  is simply a matter of contracting or expanding the space depending on whether the diffusivity takes high or low values.

In the Liouville space, Eq. (1a) and Eq. (1b) become:

$$b(\xi)pT = \frac{d}{d\xi} \left( b(\xi) \frac{dT}{d\xi} \right); \quad 0 \leq \xi < +\infty, \quad (3a)$$

$$-b(\xi) \frac{dT}{d\xi} = P; \quad \xi = 0. \quad (3b)$$

It is important to note that a *unique* variable coefficient is now present in joint Eqs. (3a)-(3b), namely  $b(\xi)$ , the profile of effusivity vs. SRDT (this would also occur with a boundary condition of third kind). The obvious consequence is that the temperature in Liouville space,  $T(p, \xi)$ , depends on  $p$ ,  $\xi$ , and this unique profile:  $b(\xi)$ ; then, the surface temperature  $T(p, x=0)$  depends only on  $p$  and  $b(\xi)$  (for the present discussion, it will not be necessary to calculate the temperature explicitly; it is sufficient to know this unique thermal dependence). The imprint of all thermal parameter profiles on the surface temperature is expressed through the profile  $b(\xi)$ ; the  $k$ - $C$  depth-profiles in Eq. 1 *have merged to reveal only this one profile,  $b(\xi)$* . The merging of the corresponding scalars, when the properties are constant, is then only a special case. This has important consequences on the identifiability of the variable thermal parameters.

### III. IDENTIFIABILITY

Effusivity clearly plays a decisive role. Indeed, it is only because of variations in effusivity with depth that the surface-temperature response differs from that of a uniform material. If there are alterations in the profiles of conductivity, VHC, or diffusivity and if these alterations do not result in a change in the effusivity profile  $b(\xi)$ , they will go unnoticed since there will be no change in the surface temperature.  $b(\xi)$  is the only property profile to which an inversion of the temperature data can give access (while applying appropriate regularization to cope with the ill-posedness of the inversion problem, but that is not the subject of this discussion). It is not possible to go further without introducing an *a priori* information.

Such information is, for example, that the compound parameter  $k^q(x)C^{q-1}(x)$ , with  $q \in \mathfrak{R}$ , is constant throughout the material (the constant value is denoted  $A$ ). With  $q = 0, 1/2$ , or  $1$  we obtain respectively a constant VHC, a constant diffusivity, or a constant conductivity. The  $\xi$ -profiles of conductivity, VHC, and diffusivity are then expressed as  $Ab^{2-2q}(\xi)$ ,  $b^{2q}(\xi)/A$ , and  $A^2b^{2-4q}(\xi)$ , respectively. All these  $\xi$ -profiles can then be rescaled to get the corresponding *depth profiles*. The latter are actually defined transitively through  $x(\xi)$ , which is obtained by inverting the Liouville variable-change in Eq. 2 while taking advantage of the fact that  $k^q(x)C^{q-1}(x)$  is constant<sup>2,3,7,8</sup>:

$$x(\xi) = \int_0^\xi \sqrt{k(\xi')/C(\xi')} d\xi' = A \int_0^\xi b^{1-2q}(\xi') d\xi'. \quad (4)$$

Since the surface temperature depends only on  $p$  and the *profile product*  $k(\xi)C(\xi)$ , the obvious consequence is that the profiles  $k(\xi)$  and  $C(\xi)$  cannot be evaluated separately without additional information. Two pairs of  $k$ - $C$  *depth-profiles* leading to the same  $\xi$ -profile  $b(\xi)$  give rise to the same temperature in Fourier-Liouville space, i.e. the same  $T(p, \xi)$  (the two corresponding distributions  $T(p, x)$  are two replicas of the same temperature distribution differently stretched along the  $x$  direction). In particular, they give rise to the same surface temperature  $T(p, x=0)$ . As a consequence, they are indistinguishable in the present thermophysical configuration. This definitely undermines the identifiability of the two-profiles inversion problem treated in Ref. 1.

To show how to construct a multiplicity of  $k$ - $C$  *depth-profiles* leading to exactly the same surface-temperature evolution, we considered the profiles in Figs. 6(a)-6(b) in Ref. 1. They each belong to  $E_x^2$ ,  $E_x^n$  being the space generated by the summation of  $n$  exponential functions of  $x$  and a constant (bulk) value (Eqs. (33)-(34) in Ref. 1). The corresponding SRDT was obtained by applying the Liouville transformation in Eq. (2), which yielded the effusivity profile  $b(\xi)$  (Fig. 1). Then, an arbitrary profile was chosen for  $k(\xi)$  or  $C(\xi)$  (i.e. the seed profile), the other being obtained from the fact that the square root of their product must be equal to the former profile  $b(\xi)$  (the only constraint is that they should be strictly positive and bounded). To start, seed profiles  $C(\xi)$  were selected in  $E_x^2$ . To translate the resulting  $\xi$ -profiles into depth profiles, we then computed  $x(\xi)$  from the left integral in Eq. 4, which yielded the conjugate  $k$ - $C$  depth-profiles shown in Fig. 2. The freedom of choice for the seed profile makes that the minimum of the profiles can be set to a completely different depth than in Figs. 6(a)-6(b) in Ref. 1; the minimum can even be changed to a maximum, see the Supplementary Material. Recall that all these conjugate  $k$ - $C$  depth-profiles lead to the same surface temperature as the profiles in Figs. 6(a)-6(b) in Ref. 1. This is a vivid illustration of the consequence of the non-identifiability of the inverse problem of simultaneous VHC and conductivity reconstruction. The conjugate profiles in Fig. 2 were built on purpose to have the same surface and bulk values as the original pair in Figs. 6(a)-6(b) in Ref. 1, thus highlighting the fact that even imposing surface and bulk values is far insufficient to make the identification unique.

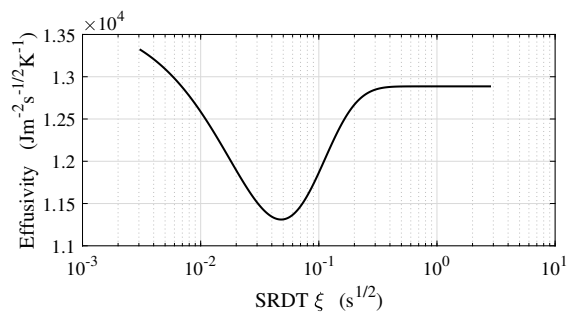


FIG. 1. Effusivity profile vs. the Square Root of Diffusion Time (SRDT)  $\xi$  inferred from the depth profiles of conductivity and VHC reported in Figs. 6(a)-6(b) in Ref. 1.

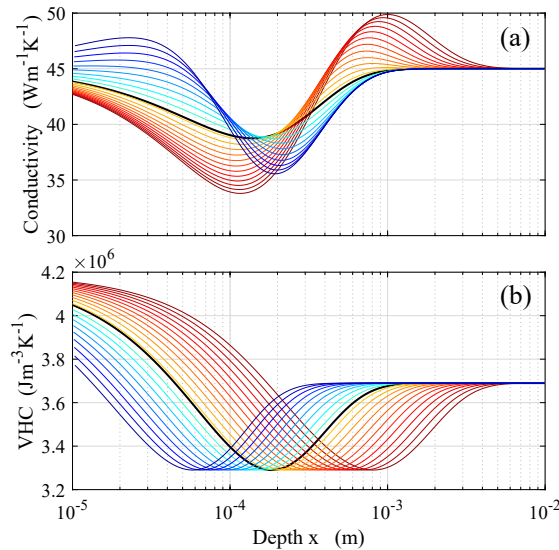


FIG. 2. Series of conjugate depth profiles of (a) conductivity and (b) VHC leading to the same effusivity profile  $b(\xi)$  shown in Fig. 1, and therefore *all giving rise to the same surface temperature*. Conductivity and VHC profiles that are conjugate have been drawn with the same color. Those from Figs. 6(a)-6(b) in Ref. 1 are in black.

#### IV. INVERSE CRIME

In Ref. 1, the inverse method was tested with  $k$ - $C$  profiles belonging to  $E_x^2$ . It may seem surprising that despite the non-identifiability nature of the inverse problem, the tests lead to profiles that are close to the profiles used to generate the synthetic temperature data. One possible explanation is that the model for  $k(x)$ , i.e.  $E_x^2$ , was the same for generating the synthetic data and for the inversion process. Using an *identical model or submodel* for both the simulation of the measurement data and the solution of the inverse problem is known to provide overly optimistic test results; this is known as *inverse crime*<sup>4</sup>. But, in fact, the reason for this unexpected success does not matter. Indeed, regardless of the inversion method used, for any (seemingly) optimal pair of  $k$ - $C$  profiles obtained by minimizing the cost function, one can find, as described above, an *infinite multiplicity* of other  $k$ - $C$  profiles giving ex-

actly the same theoretical temperature data, hence the same score for the cost function. Because these alternative solutions are not likely to belong to the (too narrow) search space (in particular  $k(x) \notin E_x^2$ ), the method used in Ref. 1 missed this huge population, and blindly converged to a solution close to the assumed pair of profiles. Among these alternative solutions, many are perfectly acceptable from the physical point of view. Finally, the non-uniqueness of the inverse problem leads to a dead end.

#### V. SUMMARY

The inverse problem presented in Ref. 1 allows to reconstruct the effusivity profile as a function of SRDT. Without independent information on the thermal properties, it is not possible to go further; thus, it is not possible to reconstruct simultaneously the conductivity and VHC depth-profiles (or the density profile if  $c(x)$  is a known constant). The Liouville transformation adds significant insights into the influence of  $k$ - $C$  profiles on the temperature response, in particular it highlights the unique role of their product (or equivalently of the effusivity), and thus reveals the full correlation of conductivity and VHC profiles. Hidden correlations must be sought, either by analytical inspection or by a sensitivity analysis, and so-called inverse crime should be avoided in order not to be misled by optimistically biased inversion tests.

#### VI. SUPPLEMENTARY MATERIAL

See supplementary material for additional figures illustrating the non-uniqueness of the considered inverse problem.

- <sup>1</sup>A. Mandelis, S. Kooshki, and A. Melnikov, "Simultaneous density and thermal conductivity depth profile reconstructions from noised thermal-wave amplitude and phase data using a combined integral-equation and imperialist competitive algorithm method," *Journal of Applied Physics* **133**, 055102 (2023).
- <sup>2</sup>J.-C. Krapez, "Thermal effusivity profile characterization from pulse photothermal data," *Journal of Applied Physics* **87**, 4514–4524 (2000).
- <sup>3</sup>J.-C. Krapez, "Heat diffusion in inhomogeneous graded media: chains of exact solutions by joint Property & Field Darboux Transformations," *Int J Heat Mass Transfer* **99**, 485–503 (2016).
- <sup>4</sup>J. Kaipio and E. Somersalo, *Statistical and computational inverse problems*, Vol. 160 (Springer Science & Business Media, 2006).
- <sup>5</sup>J. Liouville, "Second mémoire sur le développement des fonctions ou parties, de fonctions en séries dont les divers termes sont assujétis à satisfaire à une même équation différentielle du second ordre, contenant un paramètre variable," *J. Math Pures Appl.* **1**, 16–35 (1897).
- <sup>6</sup>D. Zwillinger and V. Dobrushkin, *Handbook of differential equations* (CRC Press, 2021).
- <sup>7</sup>J.-C. Krapez, "The sech( $\hat{\xi}$ )-type profiles: A Swiss-Army Knife for exact analytical modeling of thermal diffusion and wave propagation in graded media," *Int J Thermophys* **39**, 86 (2018).
- <sup>8</sup>J.-C. Krapez, "Linear, trigonometric and hyperbolic profiles of thermal effusivity in the Liouville space and related quadrupoles: Simple analytical tools for modeling graded layers and multilayers," *Int J Thermal Sci* **136**, 182–199 (2019).

## Supplementary material

# Comment on “Simultaneous density and thermal conductivity depth profile reconstructions from noised thermal-wave amplitude and phase data using a combined integral equation and imperialist competitive algorithm method” [J. Appl. Phys. 133, 055102 (2023)]

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### I. PRESENTATION

For the sake of completeness, additional figures are provided to give some more examples regarding the non-uniqueness of thermal conductivity and volumetric heat capacity (VHC) profiles, and the respective profile shapes when attempting to invert the temperature data measured on the surface of an heterogeneous material with prescribed heat flux on the same surface.

### II. FIGURES

In addition to Fig. 2 in the main text where the seed profiles  $C(\xi)$  were selected from  $E_{\xi}^2$  so as to have a single *minimum*, we also constructed a series of conjugated  $k$ - $C$  depth-profiles by selecting  $C(\xi)$  from  $E_{\xi}^2$  so as to have a single *maximum*. The profile parameters were tuned so that the maximum was set at different values of the SRDT. The bulk value for VHC was kept unchanged. A new set of conjugate  $k$ - $C$  depth-profiles is reported in colors in Figs. S1(a)-S1(b). Recall that the reference  $k$ - $C$  profiles in Figs. 6(a)-6(b) in Ref. 1 both exhibit a *minimum* (they have been reproduced in black in Figs. S1(a)-S1(b)). The new depth profiles of conductivity  $k(x)$  in Fig. S1(a) feature a local minimum as well, however, to compensate for the concavity of the VHC profiles  $C(x)$  in Fig. S1(b), while keeping the same effusivity profile in Liouville space,  $b(\xi)$ , in Fig. 1 (main text), the conductivity profiles  $k(x)$  in Fig. S1(a) have to exhibit a deeper depression as compared to the reference conductivity profile (black curve in Fig. S1(a)).

In Figs. S2 and S3, the roles of conductivity and VHC were changed as compared to Fig. 2 (main text) and Fig. S1, respectively: in Figs. S2 and S3, the conductivity was taken to provide the seed profile. In Fig. S2, the profiles  $k(\xi)$  were

selected in  $E_{\xi}^2$  while featuring a *minimum* at various values of the SRDT. To compensate for the alteration in the conductivity profile, while keeping the same effusivity profile in Liouville space,  $b(\xi)$ , the depth-profiles of VHC,  $C(x)$ , get more complex shapes as compared to the reference VHC profile reported in black, see Fig. S2(b): the new VHC profiles feature up to three local extrema, as was observed symmetrically for the conductivity depth-profiles  $k(x)$  in Fig. 2(a).

The exercise continued in Fig. S3 where, instead of featuring a single *minimum*, the seed profiles  $k(\xi)$  were chosen to feature a single *maximum*. Symmetrically to Fig. S1, the VHC depth-profiles  $C(x)$  feature a single minimum like the reference VHC profile in Fig. 6(b) in Ref. 1 and reported in Fig. S3(b) in black. However, to compensate for the concavity of the conductivity profiles  $k(x)$  in Fig. S3(a), while keeping the same effusivity profile in Liouville space,  $b(\xi)$ , in Fig. 1 (main text), the VHC profiles  $C(x)$  in Fig. S3(b) have to exhibit a deeper depression as compared to the reference VHC profile (black curve in Fig. S3(b)).

If it were still necessary to demonstrate the high diversity of the  $k$ - $C$  profiles giving rise to the same temporal evolution of the surface temperature, we provide a final example in Fig. S4 with conjugate profiles showing a wavy shape. They were constructed by choosing sinusoidal functions of  $\xi$  for the seed profile  $k(\xi)$ .

One should realize that despite large differences in shape, all of the conjugate  $k$ - $C$  depth-profiles shown in Figs. 2 (main text), S1, S2, S3 and S4, share the same effusivity profile in Liouville space (Fig. 1 - main text) and are therefore subject to the same temporal evolution of the surface temperature (whether in modulated or transient regime).

<sup>1</sup>A. Mandelis, S. Kooshki, and A. Melnikov, “Simultaneous density and thermal conductivity depth profile reconstructions from noised thermal-wave amplitude and phase data using a combined integral-equation and imperialist competitive algorithm method,” Journal of Applied Physics **133**, 055102 (2023).

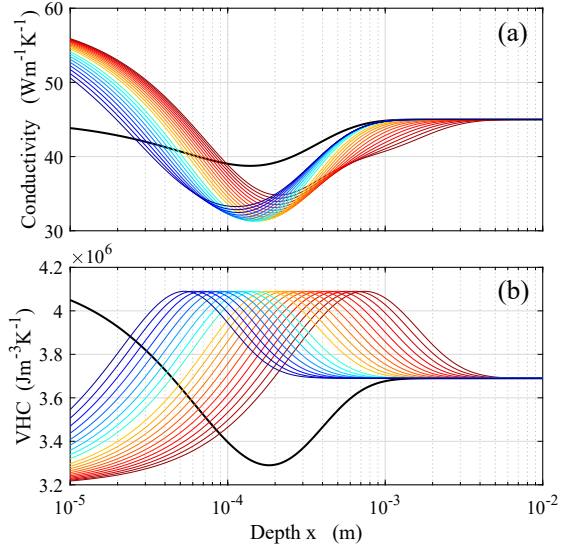


FIG. S1. Same as Fig. 2 in the main text except that here the seed profiles  $C(\xi)$  exhibit a *maximum*. They were taken in  $E_{\xi}^2$  while keeping the same bulk value as the original VHC profile in Fig. 6(b) in Ref. 1. Conjugate  $k$ - $C$  profiles have been drawn with the same color. The original  $k$ - $C$  profiles from Fig. 6(a)-6(b) are in black.

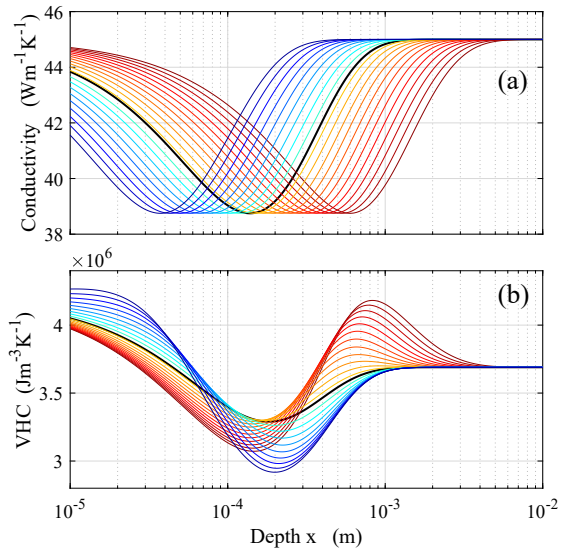


FIG. S2. Same as Fig. 2 in the main text except that here the profile to be chosen as the seed profile, is the conductivity profile. A series of  $k(\xi)$  profiles were selected from  $E_{\xi}^2$  to exhibit a *minimum* while keeping the same surface and bulk values as the original conductivity profile in Fig. 6(a) in Ref. 1.

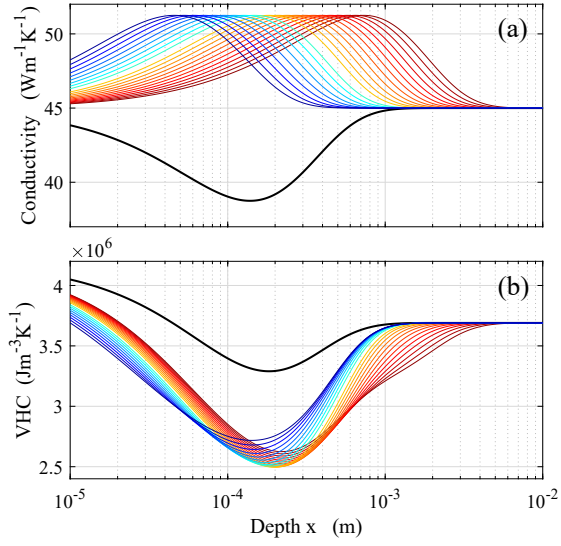


FIG. S3. Same as Fig. S2 except that here the seed profiles  $k(\xi)$  exhibit a *maximum*. They were taken in  $E_{\text{SRDT}}^2$  while keeping the same bulk value as the original VHC profile in Fig. 6(a) in Ref. 1.

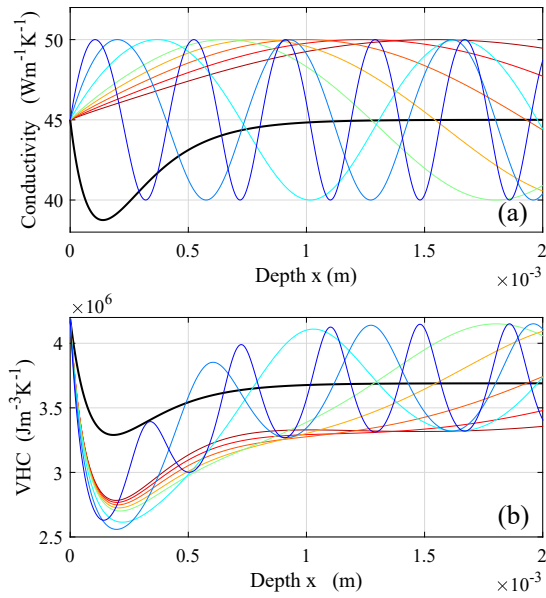


FIG. S4. Same as Fig. S2 except that here the seed profiles  $k(\xi)$  are sinusoidal functions of the SRDT with different frequency values.