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# General imperfect interfaces

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**Abstract**

The objective of this contribution is to develop a thermodynamically consistent theory for general imperfect interfaces and to establish a unified computational framework to model all classes of such interfaces using the finite element method. The interface is termed general imperfect in the sense that it allows for a jump of the temperature as well as for a jump of the normal heat flux across the interface. Conventionally, imperfect interfaces with respect to their thermal behavior are restricted to being either highly-conducting (HC) or lowly-conducting (LC) also known as Kapitza. For a HC interface the temperature is continuous across the interface while the jump of the normal heat flux is admissible. On the contrary, a LC interface does not allow for a jump of the heat flux across the interface but it does allow for a temperature jump. The temperature jump of a LC interface is frequently assumed to be proportional to the average heat flux across the interface. In this contribution we prove that this common assumption is indeed an appropriate condition to (sufficiently and not necessarily) satisfy the second law of thermodynamics.

While HC and LC interfaces are generally accepted and well established today, the general imperfect interfaces remain poorly understood. Here we propose a thermodynamically consistent theory of general imperfect interfaces and we show that the dissipative structure of the interface suggests firstly to classify such interfaces as semi-dissipative (SD) and fully-dissipative (FD). Secondly, for a FD interface the interface temperature shall be considered as an independent degree of freedom and a new (constitutive) equation is obtained to calculate the interface temperature using a new interface material parameter i.e. the *sensitivity*. Furthermore, we show how all types of interfaces are derived from a FD general imperfect interface model. This finding allows us to establish a unified finite element framework to model all classes of interfaces. Full details of the novel numerical scheme are provided. Key features of general imperfect interfaces are then elucidated via a series of three-dimensional numerical examples. In particular, we show that according to the second law the interface temperature may not necessarily be the average of (or even between) the temperatures across the interface. Finally, we recall since the influence of interfaces on the overall response of a body increases as the scale of the problem decreases, this contribution has certain applications to nano-composites.


*Keywords:* General imperfect interface; Highly-conducting; Lowly-conducting; Kapitza; Nano-materials; Finite element method

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## 1. Introduction

Interfaces within a solid can play a significant role in the overall response of a body and their influence increases as the scale of the problem decreases. (see e.g. [6,11,13, and references therein]). Furthermore the thermal properties of the interface can differ markedly from those of the surrounding bulk. Increasing applications of thermal interface materials (TIMs) on one hand (see the review paper [47, and references therein]) and unusual thermal behavior of surface and interface at the nano-scale and their applications [4,7,5,46] on the other hand motivate the task to establish a more general theory of thermal interfaces. In doing so, the standard interface theory is extended to fully energetic interfaces. The interface is assumed to be energetic in the sense that it possesses its own energy, entropy, constitutive relations, and dissipation. The governing equations for a general transient problem are provided. Interfaces can be classified according to their thermal properties as follows (summarized in Table 1).

- *Perfect interface*: The jump in the temperature and in the normal heat flux across the interface is zero. This type of interfaces are also termed *standard interfaces* or *free singular surfaces* [9].
- *Imperfect interface*: Either the temperature or the heat flux (or both) across the interface is discontinuous. Imperfect interfaces could hence be classified into three categories:
  - *HC imperfect interface*: This type of imperfect interface models has a continuous temperature across the interface, whilst allowing a jump in the normal component of the heat flux. It is shown that a heat conduction *along* the interface could lead to the jump of the normal heat flux *across* the interface. HC interfaces are also termed as *thermal interfaces*.
  - *LC imperfect interface*: This type of imperfect interface is classically modeled using Kapitza's assumption of thermal resistance. We show that this assumption is indeed in accordance with the second law of thermodynamics. The model allows for a temperature jump but not a (normal) heat flux jump across the interface.
  - *General imperfect interface*: In this general case neither the jump in the temperature nor the normal heat flux across the interface need be zero. A thermal interface is clearly an example of a general imperfect interface. General imperfect interfaces can be employed for different applications e.g. [43] developed a thermal interface suitable for cohesive zone model.

### *1.1. Key objectives and contributions of this work*

This section summarizes the key objectives and contributions of this work and more importantly the need for such a theory is motivated with recourse to the available literature on the subject.

It is enlightening to detail more on different types of interfaces introduced here (later summarized in Table 3) and their connections to available interface models. Recall, if both jumps in the temperature and normal heat flux vanish, the interface is perfect. Imperfect interfaces allow for such jumps and are bounded

Table 1
Classification of thermal interfaces.

| Interface thermal characteristic | Thermal fields | | References |
|---|---|---|---|
| | Temperature jump | Heat-flux jump | |
| Perfect | No | No | *Trivial interfaces* e.g. [9] |
| HC imperfect | No | Yes | *Stationary*: Lipton [34]; Miloh and Benveniste [37]; Duan and Karihaloo [14]; Yvonnet et al. [52]; Le-Quang et al. [31]<br>*Transient*: Javili et al. [26] |
| LC imperfect | Yes | No | *Stationary*: Hasselman and Johnson [22]; Torquato and Rintoul [50]; Lipton and Vernescu [35]; Nan et al. [41]; Duan and Karihaloo [14]; Yvonnet [53]<br>*Transient*: Javili et al. [25] |
| General imperfect | Yes | Yes | Thermodynamically consistent theory and numerical aspects using the finite element method for a fully transient problem is detailed in the current work |