# Mechanical analysis of Nanocomposites

The improvement of materials performance is a major issue in any technological field. Among others, material durability is one of the main topics under investigation, which is of critical importance in case of materials which operate under difficult situations, for instance, adverse environmental conditions, subjected to high stresses, or under repetitive loading cycles. One of the main causes of failure is the formation and propagation of cracks in the structure, processes that can be controlled and minimized by a proper design at the micro- and nano- levels.

Nanocomposites are materials which are composed by two or more phases, at least one of them with one dimension in the nanometric size. They show not only properties of the phases composing it, but also additional ones from the nano-combination of different phases. In particular, nanocomposite structures formed by a hard phase embedded in a soft lubricious matrix exhibit a combination of properties that make them very attractive for protective purposes. Among others, they show fracture toughness, high hardness, chemical inertness, low coefficient of friction and high wear resistance. However, while their tribological performance can be explained in terms of phase ratio and surface interactions, the behavior under stress is still not well understood.

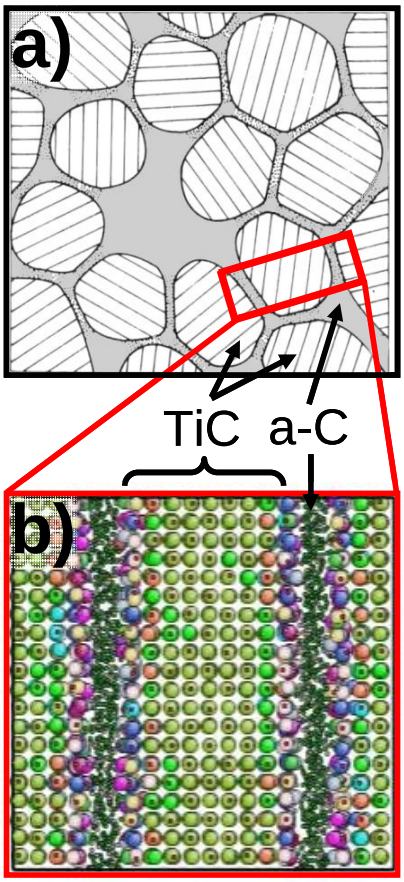


***Fig. 1.*** *a) Scheme of a nanocomposite. b) Simple simulation around a grain.*

In this project, a 'simple' system composed by TiC nanocrystals embedded in an amorphous carbon (a-C) matrix has been selected for studying this effect in detail (see Fig. 1a). This material shows good frictional performance due to the presence of a graphitic-like solid lubricant, but better

mechanical properties than a-C alone due to the presence of harder TiC nanograins. In addition, this material shows an improved toughness (capability of plastic deformation without fracture) with respect to both phases forming it. In other words, the combination of TiC and a-C at nanoscale has better much resistance to cracking than TiC or a-C alone.

Although qualitative explanations for this behavior can be found in literature, a detailed mechanism has not been described yet. We simulated the deformation by Molecular Dynamics. The simplest situation is depicted in Fig. 1b, which corresponds to a 'building block' of the whole structure (a TiC grain with the nearer a-C regions). When such system is subjected to stress (σ), a crack is formed in the a-C (which is more brittle) perpendicular to the stress direction. However, the final results are very different depending on the relative orientation of the crack and the boundaries (Fig. 2). If perpendicular, the crack is blocked by the presence of TiC, which allows maintaining the material integrity for longer (Fig. 2a). If parallel, the originated crack can propagate without restrictions and material failure occurs (Fig. 2b).

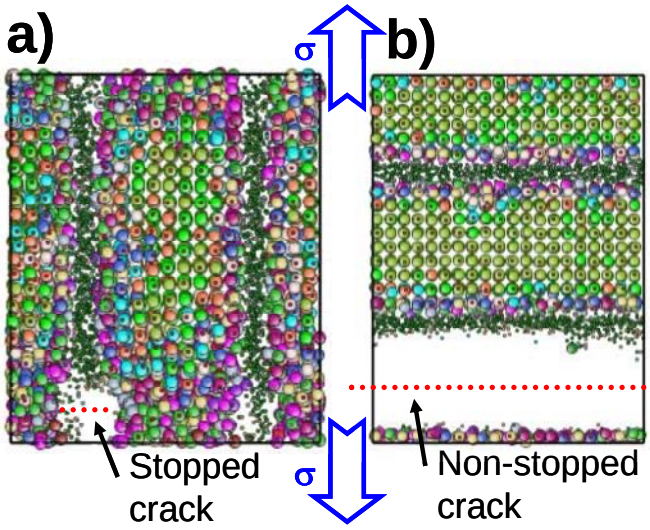


***Fig. 2.*** *Deformation of a nanocomposite in parallel (a) and perpendicular (b) directions to the grain-amorphous boundaries.*

This behavior is also observed in more complex simulations (cf. Fig. 3); the propagation of cracks generated in the a-C phase is hindered by the presence of TiC. Our approach will permit finding the optimal phase ratio and grain shape (and shape eventually) in order to achieve the highest fracture toughness of nanocomposites.

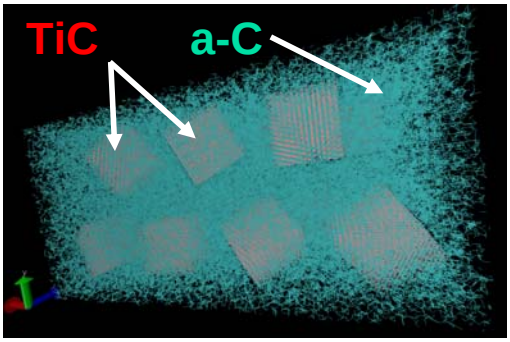


***Fig. 3.*** *Example of structure used for more sophisticated simulations.*