Mechanical properties of iron filled carbon nanotubes: Numerical simulations

Por: Munizaga, V (Munizaga, Vicente)[1,2] ; Ramirez, R (Ramirez, Ricardo)[2,3] ; Kiwi, M (Kiwi, Miguel)[2,4] ; Garcia, G (Garcia, Griselda)[3,5]

Ver ResearcherID y ORCID

JOURNAL OF APPLIED PHYSICS
Volumen: 121
Número: 23
Número de artículo: 234303
DOI: 10.1063/1.4986484
Fecha de publicación: JUN 21 2017
Tipo de documento: Article

Ver impacto de la revista

Resumen

The deformation process of Fe encapsulated in a carbon nanotube (CNT) is investigated by means of classical molecular dynamics. The [100], [110], and [111] Fe crystal orientations parallel to the CNT symmetry axis, as well as the temperature dependence, are studied. The system encompasses approximately 80 000 atoms. While crystal orientation and temperature determine the system's response, the results are almost independent of the strain rate that is applied. This behavior is only slightly modified by the Fe encapsulation in the CNT. The principal energy release mechanism is the generation of dislocations and twin boundaries, at low and intermediate temperatures (T <= 600K). The dislocations and twin boundaries interact, but do not interlock. For large temperatures (T similar to 1000K), a different reaction to deformation sets in, and no elastic response of the Fe-CNT system is observed. Published by AIP Publishing.

Palabras clave

KeyWords Plus: MOLECULAR-DYNAMICS; DEFORMATION; NUCLEATION; GROWTH

Información del autor

Dirección para petición de copias: Munizaga, V (autor para petición de copias)

Univ Diego Portals, Fac Ingn & Ciencias, Avda Ejercito 441, Santiago 8370191, Chile.

Dirección para petición de copias: Munizaga, V (autor para petición de copias)

CEDENNA, Ctr Desarrollo Nanociencia & Nanotecnol, Avda Ecuador 3493, Santiago 9170124, Chile.

Direcciones:

[1] Univ Diego Portals, Fac Ingn & Ciencias, Avda Ejercito 441, Santiago 8370191, Chile

[2] CEDENNA, Ctr Desarrollo Nanociencia & Nanotecnol, Avda Ecuador 3493, Santiago 9170124, Chile

[3] Univ Catolica Chile, Fac Fis, Casilla 306, Santiago 6904411, Chile

[4] Univ Chile, Fac Ciencias, Dept Fis, Casilla 653, Santiago 7800024, Chile

[5] CIEN UC, Ctr Invest Nanotecnol & Mat Avanza, Casilla 306, Santiago 6904411, Chile

Financiación

Entidad financiadora	Número de concesión
FONDECYT	1160639 1130272
AFOSR	FA9550-16-1-0122
CEDENNA (BASAL/CONICYT GRANT)	FB0807

Ver texto de financiación

Editorial

AMER INST PHYSICS, 1305 WALT WHITMAN RD, STE 300, MELVILLE, NY 11747-4501 USA

Información de la revista

- **Impact Factor:** Journal Citation Reports

Categorías / Clasificación

Áreas de investigación: Physics

Categorías de Web of Science: Physics, Applied