

FINITE ELEMENT ANALYSIS OF THE EFFECT OF CONTACT FORCES IN HEAT CONDUCTION OF COMPOSITE MATERIALS

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Current study uses a thermomechanical surface contact finite element formulation for analyzing interfacial heat conductance in correlation to Carbon Nanotubes contact forces. The atomic lattice of CNTs is initially modeled using the molecular structural mechanics approach and reduced to an equivalent 2D continuum element. The equivalent 2D continuum element is used as a robust and efficient surrogate model for the construction of full length CNTs in contact. Coupled structural and heat pde's have been used to describe the corresponding thermomechanical problem which are discretized using 2D quadrilateral finite elements, along with surface contact elements. The problem was solved using a Newton-Raphson incremental-iterative scheme. Extensive sensitivity analysis was performed with respect to a number of influencing parameters, such as initial contact angle, boundary conditions and CNT overlapping.

REFERENCES

- [1] Agelet de Saracibar, C. (1998). Numerical Analysis of Coupled Thermomechanical Frictional Contact Problems. Computational Model and Applications. *Archives of Computational Methods in Engineering*(5), pp. 243-301.
- [2] Balandin, A. (2011). Thermal properties of graphene and nanostructured carbon materials. *Nature Materials*, 10, pp. 569-581.
- [3] Bathe, K.-J. (2014). *Finite Element Procedures* (2nd Edition ed.). Klaus-Jürgen Bathe.
- [4] Buonanno, G., Giovinco, G., & Massarotti, N. (2003). An Elasto-plastic Model of Thermal Contact Conductance Between Nominally Flat Surfaces in Vacuum. *Int. Comm. Heat Mass Transfer*(30), pp. 921-930.
- [5] Che, J., Cagin, T., & Goddard, W. (2000). Thermal conductivity of carbon nanotubes. *Nanotechnology*(11), pp. 65-69.
- [6] Cheng, H., Chen, W., & Liu, Y. (2010). Radial mechanical properties of single-walled carbon nanotubes using modified molecular structure mechanics. *Computational Materials Science*(47), pp. 985–993.

- [7] Cooper, M., Mikic, B., & Yovanovich, M. (1969). Thermal Contact Conductance. *Int. J. Heat Mass Transfer*, 12, pp. 279-300.
- [8] Fenech, H., & Yovanovich, M. (1966). Thermal Contact Contuctance of Nominally Flat, Rough Surfaces in a Vaccum Environment. *AIAA 3rd Aerospace Sciences Meeting*, 66-42.
- [9] Konyukhov, A., & Izi, R. (2015). *Introduction to Computational Contact Mechanics: A Geometrical Approach*. Wiley.
- [10] Konyukhov, A., & Schweizerhof, K. (2013). *Computational Contact Mechanics: Geometrically Exact Theory for Arbitrary Shaped Bodies*. Springer.
- [11] Kumanek, B., & Janas, D. (2019). Thermal conductivity of carbon nanotube networks: a review. *J Mater Sci*, 54, pp. 7397–7427.
- [12] Lee, C., Wei, X., Kysar, J., & Hone, J. (2008). Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene. *Science*, 321, pp. 385-388.
- [13] GFEC. Retrieved from Github: <https://github.com/VasilisMerevis/GFEC>
- [14] Papageorgiou, D., Kinloch, I., & Young, R. (2017). Mechanical properties of graphene and graphene-based nano composites. *Progress in Material Science*, 90, pp. 75 - 127.
- [15] Peng, Z., Chen, Y., & Feng, X. (2019). A novel approach to temperature-dependent thermal contact conductance during transient isothermal cooling. *International Journal of Heat and Mass Transfer*(130), pp. 1170-1177.
- [16] Pop, E., Mann, D., Wang, Q., Goodson, K., & Dai, H. (2006). Thermal Conductance of an Individual Single-Wall Carbon Nanotube above Room Temperature. *Nano Letters*(6), pp. 96-100.
- [17] Reddy, J. N. (2005). *Introduction to the Finite Element Method* (3rd Edition ed.). McGraw-Hill Education.
- [18] Salaway, R., & Zhigilei, L. (2016). hermal conductance of carbon nanotube contacts: Molecular dynamics simulations and general description of the contact conductance. *Physical Review B*(94), p. 014308 .
- [19] Savvas, D. N., Papadopoulos, V., & Papadrakakis, M. (2012). The effect of interfacial shear strength on damping behavior of carbon nanotube reinforced composites. *International Journal of Solids and Structures*(49), pp. 3823-3837.
- [20] Tserpes, K. I., & Papanikos, P. (2005). Finite element modeling of single-walled carbon nanotubes. *Composites: Part B*(36), pp. 468–477.
- [21] Tserpes, K. I., Papanikos, P., Labeas, G., & Pantelakis, S. G. (2008). Multi-scale modeling of tensile behavior of carbon nanotube-reinforced composites. *Theoretical and Applied Fracture Mechanics*(49), pp. 51-60.
- [22] Wriggers, P. (2006). *Computational Contact Mechanics* (2nd Edition ed.). Springer.
- [23] Wriggers, P., & Miehe, C. (1994). Contact Constraints Within Coupled Thermomechanical Analysis - A Finite Element Model. *Comput. Methods Appl. Mech. Engrg.*, 113, pp. 301-309.
- [24] Wriggers, P., & Zavarise, G. (1991). Thermomechanical Contact - A Rigorous but Simple Numerical Approach. *Computers & Structures*, 46, pp. 47-53.
- [25] Yakobson, B., & Avouris, P. (2001). Mechanical Properties of Carbon Nanotubes. *Topics Appl. Phys.* 80, 80, pp. 287-327.

- [26] Yamada, Y., Nishiyama, T., Yasuhara, T., & Takahashi, K. (2012). Thermal Boundary Conductance between Multi-Walled Carbon Nanotubes. *Journal of Thermal Science and Technology*, 7, pp. 190-198.
- [27] Yovanovich, M. (1982). Thermal Contact Correlations. *Spacecraft Radiative Transfer and Temperature Control*, 83, pp. 83-95.
- [28] Yovanovich, M. (1995). Empirical Methods to Predict Vickers Microhardness. *Wear*, 193, pp. 91-98.
- [29] Yovanovich, M. (2005). Four Decades of Research on Thermal Contact, Gap, and Joint Resistance in Microelectronics. *IEEE Transactions on Components and Packaging Technologies*, 28, pp. 182-206.
- [30] Yovanovich, M., & Song, S. (1987). Explicit Relative Contact Pressure Expression: Dependence Upon Surface Roughness Parameters And Vickers Microhardness Coefficients. *American Institute of Aeronautics and Astronautics*.
- [31] Zavarise, G., Wriggers, P., Stein, E., & Schrefler, B. A. (1992a). A Numerical Model for Thermomechanical Contact Based on Microscopic Interface Laws. *Mechanics Research Communications*, 19, pp. 173-182.
- [32] Zavarise, G., Wriggers, P., Stein, E., & Schrefler, B. A. (1992b). Real Contact Mechanisms and Finite Element Formulation - A Coupled Thermomechanical Approach. *International Journal For Numerical Methods in Engineering*, pp. 767-785.