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Artificial intelligence based analysis of nanoindentation load–displacement data using a genetic algorithm

Abraham Burleigh [a], Miu Lun Lau [b], Megan Burrill [c], Daniel T. Olive [d], Jonathan G. Gigax [d], Nan Li [d], Tarik A. Saleh [d], Frederique Pellemoine [e], Sujit Bidhar [e], Min Long [b], Kavin Ammigan [e], Jeff Terry [a,c,f,*]

[a] *Department of Physics, Illinois Institute of Technology, Chicago IL 60616, United States of America*
[b] *Department of Computer Science, Boise State University, Boise ID 83725, United States of America*
[c] *Department of Mechanical, Materials, and Aerospace Engineering, Illinois Institute of Technology, Chicago IL 60616, United States of America*
[d] *Los Alamos National Laboratory, Los Alamos NM 87545, United States of America*
[e] *Fermi National Accelerator Laboratory, Batavia IL 60510, United States of America*
[f] *Department of Social Sciences, Illinois Institute of Technology, Chicago IL 60616, United States of America*

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ABSTRACT

We developed an automated tool, `Nanoindentation Neo` package for the analysis of nanoindentation load–displacement curves using a Genetic Algorithm (GA) applied to the Oliver-Pharr method (Oliver et al.,1992). For some materials, such as polycrystalline isotropic graphites, Least Squares Fitting (LSF) of the unload curve can produce unrealistic fit parameters. These graphites exhibit sharply peaked unloading curves not easily fit using the LSF, which tends to overestimate the indenter tip geometry parameter. To tackle this problem, we extended our general materials characterization tool `Neo` for EXAFS analysis (Terry et al., 2021) to fit nanoindentation data. `Nanoindentation Neo` automatically processes and analyzes nanoindentation data with minimal user input while producing meaningful fit parameters. GA, a robust metaheuristic method, begins with a population of temporary solutions using model parameters called chromosomes; from these we evaluate a fitness value for each solution, and select the best solutions to mix with random solutions producing the next generation. A mutation operator then modifies existing solutions by random perturbations, and the optimal solution is selected. We tested the GA method using Silica and Al reference standards. We fit samples of graphite and a high entropy alloy (HEA) consisting of BCC and FCC phases.

1. Introduction

Nanoindentation is a technique well suited to probing mechanical properties because it can extract hardness and elastic modulus values from very shallow regions of a sample on the order of microns. During the nanoindentation process materials undergo two types of material deformation: plastic and elastic [1]. For a fully elastic deformation, as seen in the load displacement curve of Fig. 1(a) for fused silica the material is able to fully recover its original shape (for sufficiently small indents) resulting in an unloading curve that closely traces the loading. At the other extreme, a completely plastic deformation results in an unloading curve that is nearly vertical as the material fails to recover leaving a large residual indent to nearly the full depth as shown for single crystal aluminum in Fig. 1(b).

Fine grained, isotropic graphite grades are utilized in many current and future fixed target, high-energy proton beam experiments for neutrino production [2–5]. Low-Z materials produce favorable secondary particle spectra optimal for neutrino production [5,6], and graphite offers strong resistance to thermal shock [4,7] which is a major concern for pulsed beam targets that experience a drastic increase in mechanical load due to the sharp thermal gradient during pulses. During nanoindentation some samples, such as fine grained, polycrystalline graphite, show recovery properties exhibiting regions of both elastic and plastic deformation as shown in Fig. 2 where the unloading curve is sharply peaked near the maximum load and then recovers midway through the unloading process resulting in a drastic change in the slope of the curve. This makes fitting the unloading portion of the load displacement curve difficult using a Least Squares Fitting (LSF) process as discussed in Section 2.1. Our Genetic Algorithm (GA)-based fitting process is able to fit this data accurately and efficiently while producing fitting parameters that are physically meaningful and consistent with theory.

* Correspondence to: 3101 S. Dearborn St., Chicago IL 60616, United States of America.
E-mail address: terryj@iit.edu (J. Terry).

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