LAMMPS Input Structure Generator for Functionally Graded Materials (FGM)

First-time User Guide

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Introduction to Functionally Graded Material (FGM)

Functionally graded materials (FGM) consist of two or more different materials, where the composition continuously varies along a dimension following a particular function.

With the emergence of nanotechnology, the applications of Functionally graded materials have shifted from their conventional usage towards sophisticated micro and nanoscale electronics and energy conversion devices.

Hence, we need to study FGMs in nanoscale using LAMMPS. But generating FGM structure files for LAMMPS is difficult and it is impeding the research of FGM nanostructures.

With this tool you can generate any FGM structure file with your own specifications.
Modeling Method of Generating FGM Structures

We are implementing 3 steps in modeling FGM structures:

• A structure made of material 1 atoms with specified dimensions will be generated.

• The structure will be divided into a number of small chunks of appropriate shape and thickness.

• Then material 1 atoms will be randomly replaced by material 2 atoms according to material 2’s weight fraction $f(x)$. This is called grading function. It will be discussed in next pages.
Features of This Tool

Shape of the structure:
- Cylindrical
- Cuboid
- Sphere

Grading direction:
- Radial
- Axial

Grading function:
- P-FGM (Power law function)
- E-FGM (Exponential function)
- S-FGM (Sigmoid function)
- Custom

Lattice type:
- FCC (Face-centered-cubic)
- BCC (Body-centered-cubic)

P-FGM: \( f(x) = (x)^p \)
E-FGM: \( f(x) = 1 - e^{-(x)^p} \)
S-FGM: \[
\begin{align*}
&f(x) = \frac{1}{2} (2x)^p \quad \text{for} \quad 0 \leq x \leq 0.5 \\
&f(x) = 1 - \frac{1}{2} \left(2(1 - x)\right)^p \quad \text{for} \quad 0.5 \leq x \leq 1
\end{align*}
\]

Here, \( f(x) \) is the weight percentage of material 2, \( x=r/R \) for radial grading and \( x=z/L \) for axial grading.
Bin (Chunk) Sizes and Shapes

To properly generate your desired structure, you might need to understand the binning process of the modeling FGMs.

Cylindrical and spherical structure – radial grading

Cuboid structure – radial grading

Cuboid, cylindrical structure – axial grading

Spherical structure – axial grading

Yellow portions are chunks
1. Launch the LAMMPS Structure File Generator for Functionally Graded Materials (FGM) tool

- Go to https://nanohub.org/
- Log in to nanoHUB. If you do not have a nanoHUB account then create one.
- From My Tools on nanoHUB dashboard, search for “LAMMPS Input Structure Generator for Functionally Graded Materials (FGM)” and then launch the tool.
- You can also go directly to https://nanohub.org/tools/fgmbuilder and launch the tool.
2. Inputs

This is the tool interface. You will input your specifications here.
2. Inputs

Choose if you want a cylindrical, cuboid or spherical FGM structure

If you choose cylindrical, the tool will take radius and length of the cylinder. In case of cuboid, the tool will take x, y and z length as inputs. And if you choose sphere then the tool will only take radius as input. These are geometric inputs.
2. Inputs

Now choose in which direction you want the grading.
2. Inputs

Which type of grading function do you want? We have included the widely used P-FGM, E-FGM and S-FGM. These functions have been discussed earlier. By changing the function parameter, $p$, you can generate a wide range of FGMs.

You can also use your own custom grading function by selecting ‘custom’ option.
2. Inputs

**Using custom grading function:**

Here, \( f(x) \) is the weight percentage of material 2, and \( x=r/R \) for radial grading and \( x=z/L \) for axial grading.

When entering your desired function, two important things must be ensured:

a) Octave syntax is followed while writing the function, and

b) the range of \( f(x) \) must be within 0 to 1 in the domain of \( 0 \leq x \leq 1 \).
2. Inputs

Input atomic mass of both material 1 and material 2

You can get FGM structures of either FCC or BCC

Then you will input lattice parameters of both material 1 and material 2. The lattice parameter of the FGM structure will be equal to the average of these two lattice parameters.
2. Inputs

Finally input the number of bins you want. Remember, higher the bin number, the more accurate the distribution of the FGM structure. But higher bin number will increase the computational time.

But, the thickness of the bin cannot be less than half lattice parameter. So, if your input bin number is so high that the bin size becomes lower than half lattice parameter, then the tool will automatically readjust your bin number to the maximum possible value for your structure, like this:
2. Inputs

Once you have entered all the desired specifications, click the ‘simulate’ button to generate your structure.
3. Wait for simulation results
The tool will show you a LAMMPS data file that can be directly used in LAMMPS simulation. This is your desired FGM initial structure.

You can download this file by clicking here.
4. Explore Simulation Results

You can also see the distribution profiles from this tool. You can download the plot data file or image too.

The blue curve is the distribution curve obtained directly from the grading function equation. The red one is the actual distribution curve of your generated FGM structure.

You want your actual distribution curve to follow grading function. If you see that they are very different, then try increasing bin number or increasing grading dimension.
For further detail, please check this out https://arxiv.org/abs/1911.07131

If you have any queries or feature requests, feel free to contact us at our email addresses given on first page.

Researchers should cite this work as: