

EXPERIMENTAL AND MOLECULAR DYNAMICS.
STUDYING THE THERMAL INTERACTION OF GLASS
FIBER MATERIALS

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Abstract. *This study presents an experimental and molecular dynamics (MD) analysis of the thermal interaction between glass fiber and mineral wool fiber materials. The simulations were conducted using the ReaxFF force field in the LAMMPS programming package to investigate the temperature-dependent thermal conductivity and interfacial behavior of this hybrid composite system. The results revealed that the thermal conductivity of mineral wool increases up to approximately 450–500 K due to phonon-driven transport, whereas the thermal conductivity of glass fiber decreases gradually with increasing temperature because of its stable inorganic structure. The hybrid system also undergoes volumetric expansion and exhibits non-uniform spatial heat temperature because of its stable inorganic structure irregularities and heterogeneities.*

Keywords: *Molecular dynamics, thermal conductivity, ReaxFF, interface, heat flow, special clothing, clothing package, glass cloth, mineral wool, wicking, air permeability.*

This research directly contributes to the implementation of the strategic objectives outlined in the Decree of the President of the Republic of Uzbekistan No. PF-2 of January 10, 2023, “On measures to support the activities of cotton and textile clusters, radically reform the textile and garment and knitwear industries, and further increase the export potential of the sector” [1]. It is also aligned with the Resolution No. PQ-4186 of February 12, 2019, “On measures

to further deepen the reform of the textile and garment and knitwear industries and expand its export potential” [2], Resolution No. PQ-4453 of September 16, 2019, “On measures to further develop light industry and stimulate the production of finished products” [3], as well as other relevant regulatory and legal acts in this field.

At present, particular attention is being paid to the rational and efficient use of mineral raw materials and natural resources. During his visit to the Bazalt Uzbekistan cluster in Jizzakh region on April 8, 2024, President Sh. Mirziyoyev gave instructions to further expand its activities and diversify its product range. The processing of mineral raw materials and natural resources for the production of various basalt fiber materials, and their application across different sectors of the national economy, is widely practiced in many countries, including Germany, France, Italy, and the Czech Republic. In Uzbekistan, basalt and mineral fiber materials are primarily used in the construction industry, where they are valued for their non-combustibility, thermal insulation and protection, as well as being lightweight and relatively cost-effective. These products also demonstrate high performance when applied in utilities, automotive manufacturing, oil and gas, and other sectors [4].

One of the cluster enterprises “Basfiber Treyd” is currently equipped with the necessary machinery worth USD 145 million and is in the process of establishing a production capacity of 25,000 tons of basalt fiber and fabric annually, starting from 2025. As a result, alongside meeting domestic demand, up to 90% of the manufactured products are planned to be directed toward export. Considering these developments, the creation of a special protective clothing package with high thermal resistance-designed for emergency service personnel, particularly firefighters-using locally available raw materials, and the development of an efficient technology for its production, represent urgent and highly relevant tasks.

In this study, we aim to partially address this knowledge gap by conducting a comprehensive molecular dynamics (MD) analysis of the interaction between a glass cloth composite and mineral wool fiber. This may help to partially understand the intermediate stages of the experimentally obtained results and partially bridge the gap between experiment and theoretical calculations.

In the conducted experimental research, the fire and heat-resistant layer was made of T-13 grade structural glass cloth woven with 0.3 mm thick plain yarns, the mineral fiber layer was made of thin or ultra-thin fibers with a thickness of 20 to 27 mm, a diameter of 1 to 9 μm and a fiber length of 10 to 80 mm. At the same time, a decrease in the layer thickness leads to a decrease in thermal protection, and when the thickness exceeds 27 mm, the package becomes too thick, which does not allow it to be used for sewing clothes, and also makes it difficult for the employee to move when using special clothing (Fig. 1).



Figure 1. The process of making a high-temperature protective package.

The interaction processes between the atoms of the glass cloth and the mineral wool fiber material were characterized at the atomic and molecular levels using the MD method [5] implemented in the LAMMPS software

package [6]. MD simulations are used to evaluate the equilibrium and dynamic properties of complex systems and represent a computational approach based on Newtonian equations of motion, in which the positions and velocities of N -layered atoms of a given volume are calculated over time [7]. In our MD-based modeling, the ReaxFF reactive force field parameters were used to describe the interatomic interactions between clusters [8-9].

A glass cloth model with 120,000 atoms was used as a structural model in the simulations. The initial interaction between the glass fiber and the mineral wool fiber material was studied using the ReaxFF potential (Figures 2a and 2b). Then, after combining these two materials, their thermal conductivity properties were analyzed. It should be noted that the obtained simulation models are consistent with the experimentally obtained results. In order to realistically simulate the experimental glass cloth model, periodic boundary conditions were applied along the z -direction of the model target length. Then, a mineral wool fiber material of the same size was placed on top of the glass cloth.

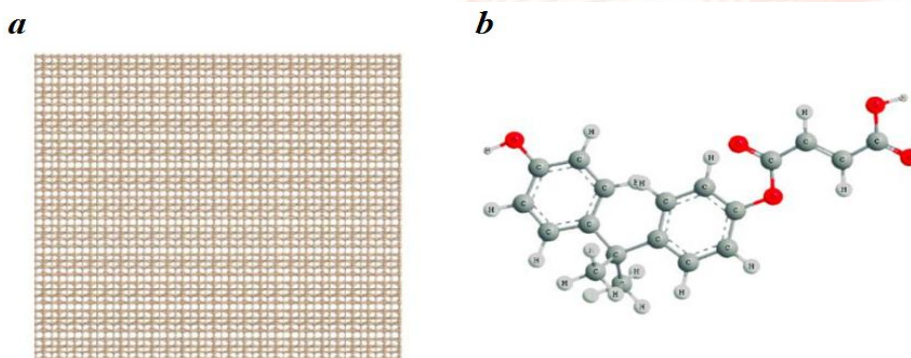


Figure 2. *a)* Appearance of a glass cloth sample. *b)* Mineral wool fiber material.

Initially, the energy of all model systems was minimized using the conjugate gradient (cg) method. Subsequently, the temperature and pressure of the systems were adjusted to the desired values (300 K) in the NpT ensemble using a Berendsen thermostat and barostat [10] with a coupling constant of 100

fs. The chosen heating rate (5 K/ps) falls within the previously reported range of 0.1–10.0 K/ps [11], with negligible deviations from thermodynamic equilibrium during the temperature ramp were negligible. For the run (100 ps), a more stringent Bussy thermostat control was used. This thermostat is based on stochastic rate shifting and provides accurate sampling from the canonical ensemble, which is well suited for the analysis of sensitive transport and diffusion properties [12]. The temperature stability was continuously monitored and remained within ± 5 K of the target temperature.

The thermal conductivity coefficient was determined using the Green-Kubo formula [13]:

$$k = \frac{1}{3Vk_B T^2} \int_0^\infty \langle J(0) \cdot J(t) \rangle dt \quad (1)$$

where V is the system volume, k Boltzmann constant, T temperature, The angle brackets $\langle - \rangle$ represent the average value of the heat flux autocorrelation function $J(t)$ over all atoms. The heat flux $J(t)$ is determined by the following formula:

$$J(t) = \frac{1}{2V} \sum_{i=1}^N \sum_{j=1}^N r_{ij} \cdot (F_{ij} \cdot v_i) \quad (2)$$

where r_{ij} and F_{ij} represent the distance and force between atoms i and j , and v_i represents the velocity of atom i .

In addition, Fourier's law expresses the relationship between the heat flux density and the temperature gradient vector [14]:

$$q = -\frac{\partial T}{\partial n} = -\lambda \text{grad} T \quad (3)$$

where q is the heat flux density and λ is the thermal conductivity, $n = \frac{\delta}{\lambda}$.

The total heat transfer rate Q for the surface area is expressed as:

$$Q = qF = -\lambda \frac{\partial T}{\partial n} \quad (4)$$

In all cases MD time step is 0.1 fs. The simulations are conducted 10 times for each study case, and the results are obtained by averaging the

corresponding physical quantities. Each simulation was repeated three times for each studied case, and the final results were obtained by averaging the individual physical quantities.

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