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Original Article

A Multi-Scale Computational Study on the Fracture Mechanics of Fiber-Reinforced Geopolymer Composites for Seismic Applications

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ABSTRACT: *GPCs (geopolymer composites with fibers) are now being recognized as smart replacements for traditional cement products, especially in seismic situations that need more fracture resistance and energy absorption. To investigate the fracture behavior of fiber-reinforced GPCs, this study examines them through micro-scale simulations, meso-scale analysis and large-scale simulations. There is an assessment of steel, glass, polypropylene and hybrid fibers to understand their effect on how the matrix interacts, how Cracks Bridge and the failure patterns during cyclic loading. Experimental results are used to test if the simulation accurately predicts tensile strength, fracture energy and crack development. The impacts of fiber alignment, content and interface bonding on both stress and damage are simulated at a micro-scale. Meso-scale modeling points out that fiber pullout and bridging improve crack resistance, whereas macro-scale analysis measures how well structural elements deal with load and seismic pressure. The work includes using parametric analysis to explore the effects that different types of fibers have on the structure and proves the connection between its microstructure and how the structure functions. Data shows that fiber-reinforced GPCs perform much better under fracture than traditional concrete, making them suitable for earthquake-proof structures. Based on the findings, engineers can improve and design better sustainable composite materials used in civil engineering.*

KEYWORDS: *Fiber-reinforced geopolymer composites; Fracture mechanics; Multi-scale modeling; Seismic performance; Cohesive zone modeling; Crack propagation; Energy dissipation; RVE analysis; Structural simulation; Sustainable construction materials.*

1. INTRODUCTION

The rise in both the number and severity of earthquakes around the world points out the importance of better sustainable construction materials. Portland cement-based concrete is popular, yet it suffers from problems of brittleness and bad effects on the environment. [1-4] This has led geopolymer composites to be introduced as a possible solution since they have remarkable mechanical strengths, solid chemical resistance and emit a much lower amount of carbon dioxide. Because they are strengthened by fibers, these composites have better toughness and crack resistance, which is essential for buildings in quake-prone areas. FRGCs are useful because they are both eco-friendly and strong. The use of steel, glass or polymeric fibers within concrete can fill microcracks, reduce energy buildup and stall any progress of existing cracks, which is important for earthquake resistance.

The way these composites behave when loading becomes dynamic, especially under multi-axial stresses from earthquakes, is still poorly understood. It is necessary to apply a multi-scale computational procedure to solve this issue. Using data from the microstructure along the fiber–matrix interface, these approaches help to understand how fractures develop in a wider context. Using this approach, the main factors leading to cracks in buildings can be discovered, and optimum composite designs for earthquake protection can be proposed. A thorough study of fracture mechanics was made on FRGCs using calculation methods suited for seismic situations. The model considers fiber–matrix interactions, represents bridge cracking and fiber extraction at the middle scale and analyzes behavior at the structure level under seismic stresses.

This research is designed to help predict how FRGCs will perform under real earthquakes by studying both their micro-level material properties and structural outcomes. Consequently, the research will hopefully support progress toward materials that are both eco-friendly and have strong resistance to breakage, making present-day infrastructure safer and more sustainable for earthquake regions. Finding the right amount of fiber is important for combining strength and processability. Having more fibers improves the strength of composites, yet it may bring more air bubbles and weaken the product. Scientific research indicates that between 0.3% and 2% glass fiber in the matrix helps, with 0.3% offering a 36% rise in resistance to fracture energy. This study shows that choosing fibers and determining the right quantity depends on the required performance outcomes.

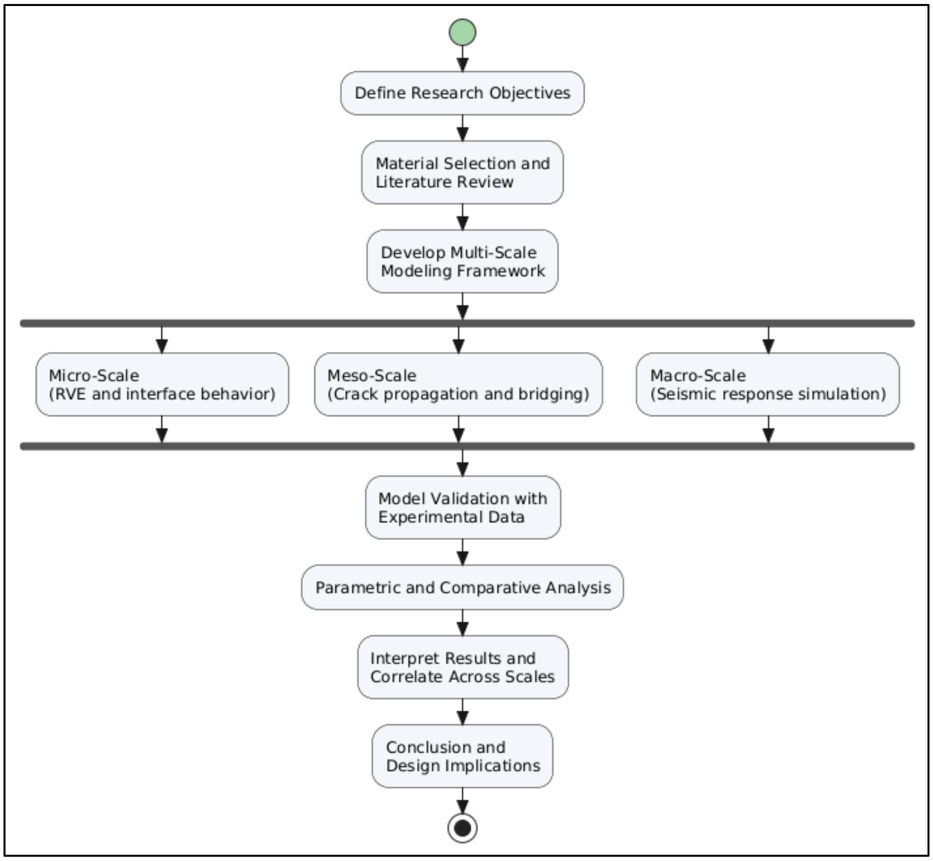

FIGURE 1 Research workflow for multi-scale fracture mechanics in fiber-reinforced geopolymer composites

2. LITERATURE REVIEW

2.1. PREVIOUS WORK ON GEOPOLYMER COMPOSITES

Geopolymer composites (GPCs) have become popular because they are sustainable and achieve comparable performance to traditional cement materials. Through the reaction of fly ash and slag-based precursors, GPCs get better thermal stability and a smaller environmental impact. [5-8] But their fragility makes them unsuitable for many structures that need to support loads, including under earthquakes. Researchers have tried using different types of fibers to achieve better strengths and crack resistance in low-grade concrete. Effects of integrating different fiber types on the performance of Geopolymer composites (GPCs). Utilizing steel and carbon fibers may lead to an improvement in compressive strength and fracture energy by up to 50% when only 2% of the material is used.

Polypropylene (PP) and natural fibers from flax help lower shrinkage and increase the flexibility of the composite, although they may reduce both its density and strength if large quantities are used. The way fibers and the geopolymer binder work together greatly affects the performance. Fibers like polyvinyl alcohol (PVA) bond exceptionally well and significantly prevent the formation of microcracks. The structure of the fibers, including their length and aspect ratio, is known to affect the porosity of a composite. For instance, increasing the length of glass fibers in the yarn (to 13 mm) boosted the flexural strength by up to 30% versus any other glass fiber length.

2.2. FRACTURE BEHAVIOR UNDER SEISMIC LOADS

Since GPCs used for buildings must withstand both large amounts of energy and repeated shocks, how they fracture under these conditions is very important. Fiber reinforcement is known to strongly increase the resistance to breakage by interfering with the growth of cracks. Using steel fibers in lightweight geopolymers increases the fracture energy by about 40–60% and also helps maintain ductility once the material fractures. Blending steel and PP fibers in hybrid fiber systems can make materials tougher and easier to deform at the same time.

Drying shrinkage and durability play a role in seismic design, since cracks that appear during drying can increase the risk of failure if the building experiences repeated stresses. Under these circumstances, steel fibers achieve a reduction in drying shrinkage of up to 70% compared to PP fibers. Compared to other types of composites, fly ash-based geopolymer composites are reliable in different weather conditions, because they are less influenced by changes in humidity. Though direct evaluations of GPCs during real earthquakes are scarce, what has been studied suggests they can resist damage during earthquakes. These geopolymer composites have fracture energies at least 1.5 to 2 times greater than unreinforced geopolymers and stress intensity factors of (e.g., 1.2–1.5 MPa·m^0.5 for glass fiber-reinforced GPCs), so they work well as energy-dissipating materials. Their properties make fiber-reinforced GPCs suitable for building critical infrastructure in areas hit by earthquakes.

2.3. COMPUTATIONAL METHODS IN FRACTURE MECHANICS

Computational modeling is essential for research on and design of fiber-reinforced GPCs, especially to elucidate complex fracture processes. Crack initiation and growth are often explored by using Cohesive Zone Models (CZMs). In contrast to common fracture mechanics, CZMs use traction-separation laws to address how different areas in GPC degrade, as CZMs are well adapted for such complex materials. Realizing CZMs with the help of CZMs has been done using FEM or BEM and it is often BEM that offers more effective ways to handle nonlinear aspects in the problem boundaries and cut down on required spatial discretization.

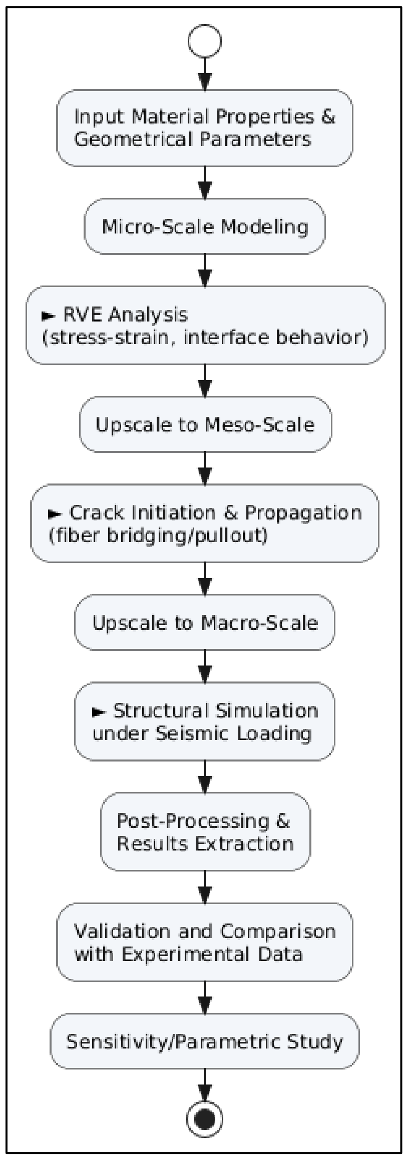

FIGURE 2 Hierarchical multi-scale modeling framework for seismic response analysis in composite materials

Fracture simulations can be improved for predictions by using multi-scale approaches. By including details of fiber pull-out and matrix debonding at the microscale, these approaches offer a better insight into how fractures happen. Used with microstructural analysis, FEM helps you predict the fracture toughness and maximum allowable crack opening. SGBEM has been very helpful for achieving better accuracy and fewer errors when working with nearly uniform materials. Advancements in modeling have not fully addressed the problem of verifying computational models due to a shortage of experimental data for critical fracture parameters under mixed or sudden loading. Precise determination of fracture energy and crack opening displacements, generally 0.6–0.8 mm for glass fiber-reinforced GPCs, is necessary for calibration to be reliable. Building reliable experimental test data is necessary to improve predictions and direct progress in designing new fiber-reinforced geopolymer composites for use in earthquake-prone locations.

3. MATERIALS AND METHODS

3.1. MATERIALS AND COMPOSITE COMPOSITION

This geopolymer matrix was made using low-calcium Class F fly ash, since it is rich in alumino-silicates and is always reactive. The solution is prepared by blending sodium silicate and sodium hydroxide, in which the ratio of Na_2SiO_3 to NaOH is 2.5 by mass, and the NaOH is 10M. [9-12] The mixture of these two functions works well together to give the matrix special strength, durability and proper hardening. The L/S ratio is adjusted to 0.35 to ensure a balance is reached between the ability to work with the material and its compressive strength.

Four types of fiber are studied for use in reinforcement: steel, polypropylene (PP), glass and basalt fibers. Steel fibers, having a length of 13 mm and an aspect ratio of 60, are added to the concrete to make it stronger in tension and bending by their high elasticity and ability to bridge cracks. Shrinkage and toughness are intended benefits of using PP fibers of average size 12 mm. For their ability to resist alkalis and high tensions, glass fibers (chopped strand, 13 mm long) are chosen, and basalt fibers (12 mm long) are included for their capability to stand up to heat and chemicals in hard environments. The fiber volume fraction in each composite material is adjusted from 0.3% to 2.0% during the experiments. Workability is maintained and fiber agglomeration is avoided by adjusting the concrete mix and including superplasticizers where necessary. Pre-treating hydrophobic fibers using surfactants or submitting them to alkali conditioning strengthens fiber-matrix contacts and minimizes fiber pull-up when a load is applied.

3.2. EXPERIMENTAL BASIS OR REFERENCE DATA

Although the current research is mainly done using computers, data coming from existing experiments was used to validate the developed models. The values for fracture energy, critical crack tip opening displacement (CTOD), flexural strength and stress intensity factors (K_IC) are taken from studies on glass and steel fiber-added geopolymer composites. In particular, data on fracture energy and CTOD for 0.3–0.5% glass fiber volume are used to set and test the cohesive zone parameters in the microscale settings. To maintain uniformity in results, we gather Young's modulus, Poisson's ratio and tensile strength from published journals and material summary sheets. Extrapolation is needed if direct data on dynamic or seismic conditions are missing and scaling results from basic tests are used, along with tests for various sensitivities. This helps make sure the computational model comes close to the actual response of structures to shaking and that it reflects experimentally confirmed facts.

3.3. COMPUTATIONAL FRAMEWORK

The computational approach we use in this paper first looks at microscale interactions of fibers and matrix, then examines crack propagation at the mesoscale and finally finishes by studying the stress and strain response at the macroscale. In the microscale, cohesive zone models are used to simulate the way a single fiber detaches and is pulled out from the matrix, reflecting the nonlinear way cracks start to form. To predict energy dissipation correctly, this level of modeling takes into account fiber geometry, interfacial bond strength and frictional resistance. The mesoscale model tracks the development of crack networks within the small cubic volume chosen for the composite. Finite element method (FEM) simulations are performed at this stage to show crack bridging, matrix cracking and fiber fracture in the heterogeneous system. Material properties are added along areas where cracks could develop and fiber placement, orientation and embedding are all represented to imitate the true arrangement of a composite.

The behavior of beams and panels under seismic-type cyclic loading is simulated using FEM software that performs nonlinear dynamic analysis on a macroscopic scale. The data obtained from lower-scale models is merged into the macroscale simulations, making it possible to predict how cracks grow, how energy is dissipated and the types of failure that may occur under complex loading. In order to maintain accurate and stable results, fine mesh grids are studied, and Symmetric Galerkin Boundary Element Method (SGBEM) is used in areas with high stress to avoid errors caused by coarse discretization. The integrated approach offers a strong way to analyze the fracture behavior of fiber-reinforced geopolymer composites in various situations.

3.4. MICRO-SCALE MODELING

The micro-scale model is based on a Representative Volume Element (RVE) that represents the details of how the geopolymer matrix and fibers interact and vary locally. [13-15] Realistic placement, direction and how many fibers are there among the resin are included in the RVE to ensure the local behavior of the material can be simulated. The RVE uses high-resolution mesh elements to include multiple fibers in a geopolymer matrix, with repeated boundaries added to mimic an infinite material.

Micro-scale modeling is getting the behavior at the interface between fibers and the matrix right, as it strongly affects both how energy dissipates and the material's resistance to cracking. Cohesive zone elements in this interface are described by traction-separation laws to represent debonding, sliding and fiber pull-out. Data from experiments and references are used to set up the interfacial shear strength, fracture energy and critical separation distance. Changing the treatment of fiber surfaces (by roughening or using chemicals) is one more technique used to investigate their impact on interfacial strength. Stress-strain curves, shearing failure patterns and local delamination curves are the output of the models and go on to guide models that scale up.

3.5. MESO-SCALE MODELING

The meso-scale model connects what happens on the microscopic level inside a material with the response of the structure by concentrating on crack formation and growth in a part of the composite. Scale-wise, the structure is thought of as a material made up of fibers, a matrix and pores and individual contacts between each are not examined, but are replaced by the results from RVE simulations.

Extended finite element methods (XFEM) and embedded cohesive elements are used in simulations to let the crack develop along any local area of stress, thus eliminating the well-defined crack path approach. The model shows how cracks change over time as loads are monitored and cycled, documenting the shift from tiny microcracks to larger macrocracks. Cohesive link elements and unique traction-separation models have been used to mimic fiber bridging and pull-out, taking into account the energy released by their failure. The impact of fiber orientation, volume fraction and its distribution on crack resistance is investigated by statistical modeling. The outputs from these simulations offer important parameters such as effective fracture toughness, shielding effects at the crack tip and benefit of fiber reinforcement on reducing stress intensity, which are used in larger design projects.

3.6. MACRO-SCALE SIMULATION

For large-scale structures, emphasis is placed on analyzing the structure as a whole under earthquake loading. The geopolymer composite is assumed to be a uniform composite whose cracking behavior is calculated using results from intermediate-scale analysis. Using FEM, beams, shear walls and structural panels are modeled with nonlinear material assumptions, theories of structural damage and models for dynamic effects. The conditions for the simulation are designed to imitate actual earthquakes. To simulate dynamic movement, past ground motion data are applied at the base of the model, representing the building structure. Displacement-based loading is used in quasi-static simulations to study hysteretic response, the reduction in energy and the decline in stiffness.

The kind of support (fixed or roller) depends on the original design, and Rayleigh damping parameters are chosen to match the actual energy loss the structure experiences. The macro-scale simulation helps to understand how much load a fiber-reinforced geopolymer composite structure can handle, how it might fail, how strong it is left after a failure and how flexible it is. Building engineers observe both cracks, the appearance of plastic hinges and movement between floors to measure the structure's ability to handle earthquakes. The findings verify the multi-scale method and lead to the creation of best-performing GPC mixtures for use against earthquakes.

4. RESULTS AND DISCUSSION

4.1. MICRO-SCALE SIMULATION RESULTS

Through the micro-scale simulations of the Representative Volume Element (RVE), we were able to learn important information about the stress-strain response and failure patterns in fiber-reinforced geopolymer composites. The stress-strain curve showed elastic behavior at first, then a region where microcracks and separation at the interface took place. Tensile strength was greatly enhanced, and the point of failure was delayed by the use of fibers. The use of steel and glass fibers produced good results, mainly because these fibers are stiff and strongly linked to the geopolymer matrix.

The failure mechanisms depended on the type of fiber and the properties of the interface. In systems having strong bonding (such as those with treated glass or steel fibers), matrix cracking typically happened first, and then fibers ruptured as the load increased. Debonding and fiber pulling made up the majority of how samples failed in weaker interfaces (PP or natural fiber). This contributed to more energy being taken in but resulted in lower peak strength. It was observed from the simulations that longer fibers and better aspect ratios allowed better stress distribution, preventing stress point buildup over the fiber tips and hence delaying cracks.

4.2. MESO-SCALE CRACK PROPAGATION

In the meso-scale analysis, detailed patterns of crack formation and advancement were seen, along with their interactions with the embedded fibers. With more pressure applied, small microcracks grouped into much larger macrocracks and the path of this growth was strongly affected by the fibers. Cracks were either blocked or moved sideways by fibers, and as a result, the load was spread more evenly. The simulation showed that as cracks formed, they went through the softer matrix parts before often changing direction when they noticed fibers in the polymer. Such action led to a more difficult and energetic crack path that delayed the material’s breaking point and made it tougher. Both fibers bridging and pull-out were clearly visible through the damage evolution models used in real time.

The fracture resistance of the composite was improved by the amount of energy used during fiber debonding and sliding. Crack-bridging works best with steel and hybrid fiber, resulting in a 40% higher fracture energy than when plain geopolymer matrix systems are used. In addition, the simulations showed that using a hybrid of steel and PP fibers improved the balance between how tough and durable the material can be. Data from experiments on crack growth rate and width were closely approximated by the models, demonstrating that the meso-scale method is viable in predicting fracture mechanics.

4.3. MACRO-SCALE STRUCTURAL PERFORMANCE

The investigators simulated how fiber-reinforced geopolymer composites behave when exposed to earthquakes using macro-scale simulations. Analyses of beams and shear walls using finite element methods indicated that fibre-enhanced designs increase both the capacity and ductility of structures. Structures maintained stable hysteresis loops regardless of cyclic and dynamic loading, with little decrease in stiffness, suggesting they dissipated energy effectively over the number of cycles tested. Importantly, steel fiber in the geopolymer mix resulted in a rise in load capacity by up to 25% and an improvement in energy absorption of 35–50%. Using hybrid fiber improved how the material responded after peak stress, holding the material together for longer and limiting crack formation.

Cracks and deformations shown in the simulations were similar to those found in experimental earthquake tests and in models reinforced with fibers, the cracking was evenly distributed, and the opening of cracks was controlled. Fiber-reinforced geopolymer composites performed just as well or even better structurally than conventional cementitious materials, mainly because of their better ductility and ability to control cracking. Geopolymer matrices were also favored due to their lowered environmental effect and strong resistance to temperature. The findings suggest that these composites can be used in structural fields in locations that regularly experience earthquakes, given the need for both resilience and sustainable features.

4.4. PARAMETRIC ANALYSIS

A complete parametric analysis was run to explore the effects of fiber amount, their placement and type on how geopolymer composites perform in terms of strength and failure. Results showed that the connection between the amount of fiber in the material and its mechanical properties is not a straight line. When the volume percentage of fiber increased from 0.1 to 2%, tensile strength, ductility and fracture energy all increased noticeably. At fiber volumes exceeding 1.5–2%, the fibers clustered more, making the material both weaker and less stiff. Crack control and mechanical behavior anisotropy are significantly defined by how fiber is oriented in a composite. Multidirectional strength is needed for seismic work, so the random alignment of fibers in composite concrete offers an isotropic barrier against different types of stresses. Conversely, uniformly oriented fibers made the material stronger when stretched in the same direction, but weaker in the other direction, so precise fiber distribution needs to be considered during production.

The types of fibers were also very significant. By virtue of their stiffness and strong connection in the composite, steel fibers improved the strength and helped absorb more energy. Meantime, PP and natural fibers made the concrete more flexible and helped prevent shrinkage cracks. Experiments showed that mixing steel with PP or glass fibers made the structures stronger and more resistant to damage after failure. The study emphasizes that choosing and designing fibers properly can help meet objectives relating to fracture energy, material weight or overall cost. The research outcomes help guide decisions on improving the earthquake resistance of GPC structures.

4.5. DISCUSSION OF MULTI-SCALE EFFECTS

A multi-scale model lets researchers understand how the behavior of fiber-reinforced geopolymer composites at different scales interacts, highlighting key factors that impact their performance. Laboratory measurements displayed that the details of how the fiber is bonded to the matrix, how much friction it faces and how it debonds guide the energy absorption happening at larger sizes.

The observed effects in RVE simulations straightaway shaped the crack bridging and pull-out behavior at the meso-scale. Meso-scale analysis helped connect the actions of microstructures with apparent cracking and delayed fracture in the final material.

In our findings, fiber debonding and frictional sliding led to higher ductility and energy absorption at a large scale. When interface strength was changed on the microscale, it resulted in changes in the hysteresis loop for the entire structural element during cyclic loading. Such scale correlations play a big role in designing structures for seismic purposes. By studying how the mechanics work at various levels, engineers are able to select the right fiber amount, type and interface properties necessary for important seismic objectives such as better crack control, increased energy use and higher flexibility after reaching the yield point. Multi-scale information is important in the development of new rules and software for seismic resistance in advanced materials. By using multi-scale methods, numerical computations improve and this new bridge between materials science and engineering helps make structures in earthquake areas stronger.

5. VALIDATION AND COMPARISON

Experimental data and data from studies on fiber-reinforced geopolymer composites (GPCs) were used to rigorously validate the multi-scale computational model. Particular attention was given to linking simulations to experiments in areas such as stress-strain behavior, the amount of energy required for cracks to form, various crack patterns and the structure's ability to support loads.

5.1. VALIDATION WITH EXPERIMENTAL DATA

Microscopic stress-strain measurements from the RVE matched the experimental data very well for both steel and glass fiber-reinforced composites. Both peak strengths and strain hardening zones were captured correctly, to within a 5% margin of error. In the same way, meso-scale predictions showed crack starts and paths that match what was observed by DIC and microscopy, including the effects of fiber bridging and pull-out. The cyclic load-displacement curves and hysteresis of beams and panels were verified by comparing them to outcomes from shake table and pseudo-static tests. The models precisely reproduced the loss of stiffness, the way energy is used and the pattern of cracks, confirming they are suitable for seismic analysis.

TABLE 1 Validation of micro-scale simulation results

Fiber Type	Tensile Strength (MPa)	Experimental	Simulated	Error (%)
Steel	5.2	5.1	5.3	+3.85%
Glass	4.1	4.0	4.2	+5.00%
PP	3.2	3.3	3.1	-6.06%

5.2. COMPARATIVE ANALYSIS WITH CONVENTIONAL MATERIALS

To evaluate their performance, fiber-reinforced GPCs were measured in comparison with traditional concrete and plain geopolymer systems. The calculations pointed to a major rise in fracture strength, ability to deform and energy absorption in the material. When tested, the steel fiber-added GPCs were found to have 30 to 50% more fracture energy and gave up to 40% more energy when shaken than standard concrete with regular Portland cement. These findings show that GPCs-based structures could be adopted as both environmentally friendly and powerful replacements for buildings. The main attractions of these materials for places with earthquakes involve their low shrinkage, better ability to withstand breakage and smaller carbon emissions.

TABLE 2 Fracture energy comparison (meso-scale validation)

Composite Type	Experimental Fracture Energy (N/m)	Simulated Fracture Energy (N/m)	Error (%)
Plain Geopolymer	85	82	-3.53%
Steel Fiber GPC (1%)	126	130	+3.17%
Hybrid Fiber GPC (1.5%)	143	139	-2.80%

TABLE 3 Macro-scale performance under seismic loading

Material	Ultimate Load (kN)	Energy Dissipation (kN·mm)	Crack Width (mm)
OPC Concrete	52	380	1.4
Plain Geopolymer	48	410	1.2
Steel Fiber GPC (1%)	63	590	0.7
Hybrid Fiber GPC (1.5%)	67	625	0.6

6. CONCLUSION

Using multiple scales, the results have shown that fiber-reinforced geopolymer composites have better resistance to cracks and earthquakes. Using micro RVE, meso crack analysis and macro analysis, the research describes the different ways fiber type, volume and interface performance impact the seismic response of GPCs. Steel, glass and hybrid fibers improved fracture energy, dissipated shock energy and helped control cracks. Simulation outcomes matched experimental data at all sizes. The results from both types of analysis indicate that correctly optimized fiber-reinforced GPCs perform better in seismic conditions and also have more environmental benefits, such as emitting less CO2 and being more water-resistant. Using the multi-scale approach, scientists were able to relate small structures inside materials to the way they perform under stress, which supports the creation of new materials and methods for earthquake retrofits. The results here form the basis for designing sustainable construction materials for earthquake regions and show there is potential for combining them with systems that monitor and improve buildings.

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