

Description:	<i>Material simulation and modeling Material and process development</i>
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### **Introduction and scope**

In recent years thermotropic overheating protection glazings are in focus of interest both, in solar thermal collector technology and architectural design of buildings. A thermotropic glazing changes its light transmittance from highly transparent to light diffusing upon reaching a certain threshold temperature autonomously and reversibly [1, 2]. Among different thermotropic systems, especially thermotropic systems with fixed domains (TSFD) are considered to have the highest potential for practical application [3, 4]. In TSFD scattering domains are embedded in a polymer matrix, which exhibit a sudden change of the refractive index upon reaching the threshold temperature. At low temperatures the layer is translucent, as the refractive indices of matrix and domain are almost equal. If the difference of the refractive index of both components increases due to warming up to a determined temperature (switching threshold) the thermotropic film turns opaque [1, 3, 5]. However, the overheating protection performance of TSFD produced so far is limited and only moderate light shielding efficiency was achieved [4, 6, 7]. Thus, within the scientific research project “Smart Windows – Smart Collectors: Development, Modeling and Application Demonstration of Overheating Protection Glazings for Facades and Solar Thermal Collectors” (funded by the State Government of Styria, Department Zukunftsfonds (project number 5019)) a systematic investigation of the effects of the refractive index difference, scattering domain parameters and the layer thickness on the overheating protection performance of TSFD was carried out on the one hand. Aim was to evaluate the theoretical light shielding potential of TSFD. Based on assessed ideal material parameters TSFD were developed, characterized and optimized systematically based on sound polymer physics on the other hand.

### **Theoretical modeling of light-shielding efficiency of TSFD**

Light shielding characteristics and potential of TSFD were studied by applying simulation of light scattering in particle filled layers. In random walk simulations numerous parameters were varied systematically and the effect on the light transmittance of TSFD was studied. Parameters included index of refraction of both the matrix material and the scattering domain, concentration of the scattering domains, and thickness of the scattering layer. The simulations demonstrated that there is great potential for the production of TSFD with excellent overheating protection performance. TSFD exhibit adequate light-shielding efficiency (90% transmittance in clear state, 40% transmittance in scattering state) if they are prepared by applying

appropriate material formulation and a tailored layer thickness, provided spherical scattering domains with diameters between 200nm and 400nm. Details are found in:

*Gruber, D.P., Winkler, G., Resch, K. (2014). Comprehensive evaluation of the theoretical light shielding potential of TSFDs for material development and optimization, submitted to Solar Energy Materials and Solar Cells.*

## Development and optimization of TSFD

TSFD were developed by applying a systematic material formulation and characterization strategy. Various matrix materials (thermoplastics, thermosets) and additives as scattering domains (paraffin waxes, fatty acids and their derivatives, polymers) were used. In total 41 different TSFD were investigated. Relationships between thermo-refractive properties of TSFD constituents, internal material structure (morphology), and light-shielding efficiency of TSFD were studied. Although thermo-refractive properties of TSFD constituents were sufficient in order to achieve efficient overheating protection performance, light shielding characteristics of produced TSFD were moderate. This was mainly ascribed to inappropriate shape and/or size of scattering domains and – to a less extent – to defects. Polymer-physical effects triggering scattering domain size/shape and defect formation were identified. Based on these results TSFD were optimized systematically. Focus was on TSFD based on UV-curing acrylate resins. Defects were prevented by optimization of processing conditions (radiation dose and intensity) and material formulation (reactive diluent, photo initiator). Adjustment of scattering domain size and shape was done via a specifically developed photo-initiated miniemulsion polymerization mediated encapsulation process for the additive. TSFD formulated with the encapsulated additive exhibited significantly improved overheating protection performance. Solar hemispheric transmittance was around 73 and 49% below and above the switching threshold, respectively. Details are found in:

*Weber, A., Resch, K. (2014). Thermotropic glazings for overheating protection. I. Material preselection, formulation, and light-shielding efficiency, Journal of Applied Polymer Science 131 (4), doi: 10.1002/app.39950.*

*Weber, A., Schmid, A., Resch, K. (2014). Thermotropic glazings for overheating protection. II. Morphology and structure-property relationships, Journal of Applied Polymer Science 131 (4), doi: 10.1002/app.39910.*

*Weber, A., Schlögl, S., Resch, K. (2013). Effect of Formulation and Processing Conditions on Light Shielding Efficiency of Thermotropic Systems with Fixed Domains Based on UV Curing Acrylate Resins, Journal of Applied Polymer Science 130, 3299-3310.*

*Weber, A., Resch, K. (2014). Thermotropic Overheating Protection Glazings: Effect of Functional Additives and Processing Conditions on Light-Shielding Efficiency, Journal of Polymer Engineering 34 (2), 161-172.*

*Weber, A., Resch, K. (2014). Thermotropic systems with fixed domains exhibiting enhanced overheating protection performance, Journal of Applied Polymer Science 131 (12), doi: 10.1002/app.40417.*

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- [2] A. Seeboth, J. Schneider, A. Patzak, Materials for intelligent sun protecting glazing, *Sol. Energy Mater. Sol. Cells* 60 (3) (2000) 263-277.
- [3] K. Resch, G. M. Wallner, Thermotropic layers for flat-plate collectors – a review of various concepts for overheating protection with polymeric materials, *Sol. Energy Mater. Sol. Cells* 93 (1) (2009) 119-128.
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