



MODEL KLASIFIKASI SISTEM KRISTAL DARI MATERIAL POLIMER BERBASIS RESNET-1D MENGGUNAKAN DIFRAKSI SINAR-X

Naufal Suryo Saputro
21/477237/TK/52557

Diajukan kepada Departemen Teknik Nuklir dan Teknik Fisika Fakultas Teknik
Universitas Gadjah Mada pada tanggal 5 November 2025
untuk memenuhi sebagian persyaratan untuk memperoleh derajat
Sarjana Program Studi Teknik Fisika

INTISARI

Analisis difraksi sinar-X (XRD) merupakan metode utama dalam karakterisasi struktur kristal material. Namun, pendekatan konvensional berbasis *search match* memiliki keterbatasan karena membutuhkan intervensi manual, bergantung pada keahlian pakar, serta kurang efisien dalam penanganan *dataset* berukuran besar. Permasalahan ini semakin menonjol pada material polimer yang menunjukkan pola difraksi kompleks akibat keberadaan fasa kristalin dan amorf secara bersamaan. Penelitian ini bertujuan mengembangkan model klasifikasi sistem kristal polimer berbasis pembelajaran mendalam dengan arsitektur ResNet-1D untuk meningkatkan akurasi dan efisiensi analisis XRD.

Dataset terdiri atas 10.948 difraktogram konversi dari berkas CIF polimer serta data eksperimen XRD pada *recycled polypropylene* (rPP) dengan tujuh variasi perlakuan. Data melalui tahapan pra-pengolahan (koreksi latar, normalisasi, *resampling*) dan augmentasi berbasis fisis (penambahan derau Gaussian, penskalaan intensitas, dan pergeseran puncak). Model ResNet-1D dengan blok residual dan mekanisme *squeeze-and-excitation* dilatih menggunakan strategi *single-seed* dan *ensemble multi-seed* dengan *test-time augmentation* serta kalibrasi probabilitas.

Model tunggal dengan augmentasi mencapai akurasi 0,82 pada data konversi dan mengklasifikasi seluruh sampel rPP dengan benar. Model *ensemble* memperoleh akurasi 0,83 serta performa sempurna pada data eksperimen. Kombinasi ResNet-1D, augmentasi data, dan strategi *ensemble* terbukti efektif mengurangi domain gap antara data konversi dan eksperimen.

Kata kunci: Difraksi sinar-x, polimer, klasifikasi sistem kristal, augmentasi data, ResNet-1D, pembelajaran mendalam

Pembimbing Utama : Prof. Ir. Nazrul E., S.T, M.T., Ph.D., IPM., ASEAN Eng.
Pembimbing Pendamping : Dr.-Ing. Ir. Kusnanto





1D-RESNET BASED CLASSIFICATION MODEL FOR CRYSTAL SYSTEMS OF POLYMER MATERIALS USING X-RAY DIFFRACTION

Naufal Suryo Saputro

21/477237/TK/52557

Submitted to the Department of Nuclear Engineering and Engineering Physics
Faculty of Engineering Universitas Gadjah Mada on November 5, 2025
in partial fulfillment of the requirement for the Degree of
Bachelor of Engineering in Engineering Physics

ABSTRACT

X-ray diffraction (XRD) is a fundamental technique for characterizing the crystal structure of materials. However, conventional search match methods are constrained by manual intervention, dependence on expert knowledge, and inefficiency in handling large datasets. These challenges are more evident in polymers, which often display complex diffraction patterns due to the coexistence of crystalline and amorphous phases. This study develops a deep learning-based classification model for polymer crystal systems using a ResNet-1D architecture to improve both accuracy and efficiency of XRD analysis.

The dataset comprises 10,948 simulated diffractograms generated from polymer CIF files and experimental XRD data from recycled polypropylene (rPP) with seven treatment variations. Preprocessing involved background correction, normalization, and resampling, followed by physics-based augmentation through Gaussian noise, intensity scaling, and peak shifting. The ResNet-1D model with residual blocks and a squeeze-and-excitation mechanism was trained using single-seed and ensemble multi-seed strategies with test-time augmentation and probability calibration.

The single model with augmentation achieved 0.82 accuracy on simulated data and correctly classified all rPP samples. The ensemble model reached 0.83 accuracy and perfect experimental performance. The integration of ResNet-1D, data augmentation, and ensemble learning effectively reduces the domain gap between simulated and experimental XRD data, establishing a robust framework for polymer crystal system classification.

Keywords: X-ray diffraction, polymers, crystal system classification, ResNet-1D, data augmentation, deep learning

Supervisor : Prof. Ir. Nazrul Effendy, S.T, M.T., Ph.D., IPM., ASEAN Eng.

Co-supervisor : Dr.-Ing. Ir. Kusnanto

