

RamPINN: Recovering Raman Spectra From Coherent Anti-Stokes Spectra Using Embedded Physics

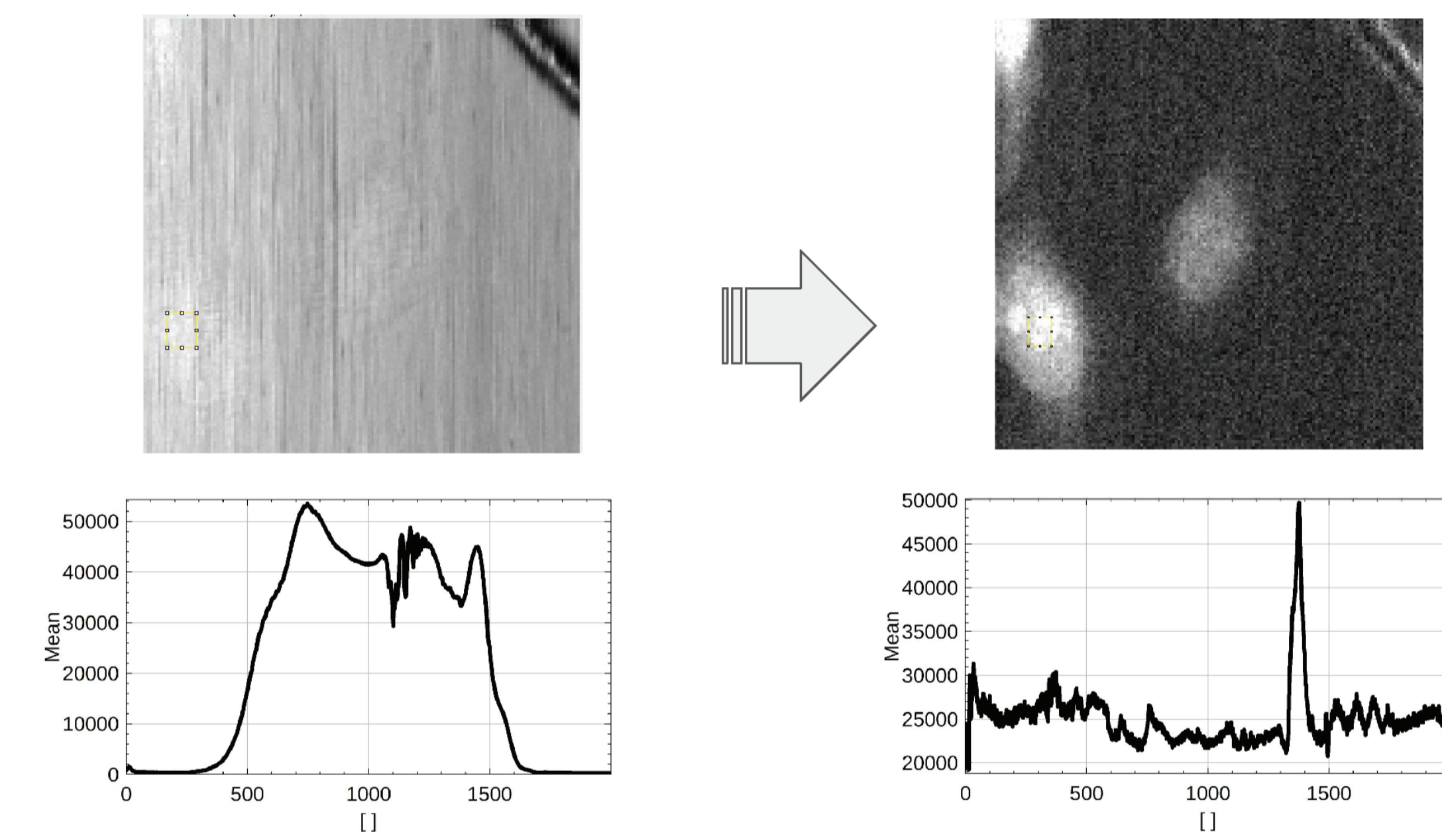


Sai Karthikeya Vemuri, Adithya Ashok Chalain Valapil, Tim Büchner, Joachim Denzler
Computer Vision Group, Friedrich-Schiller-University Jena, Germany



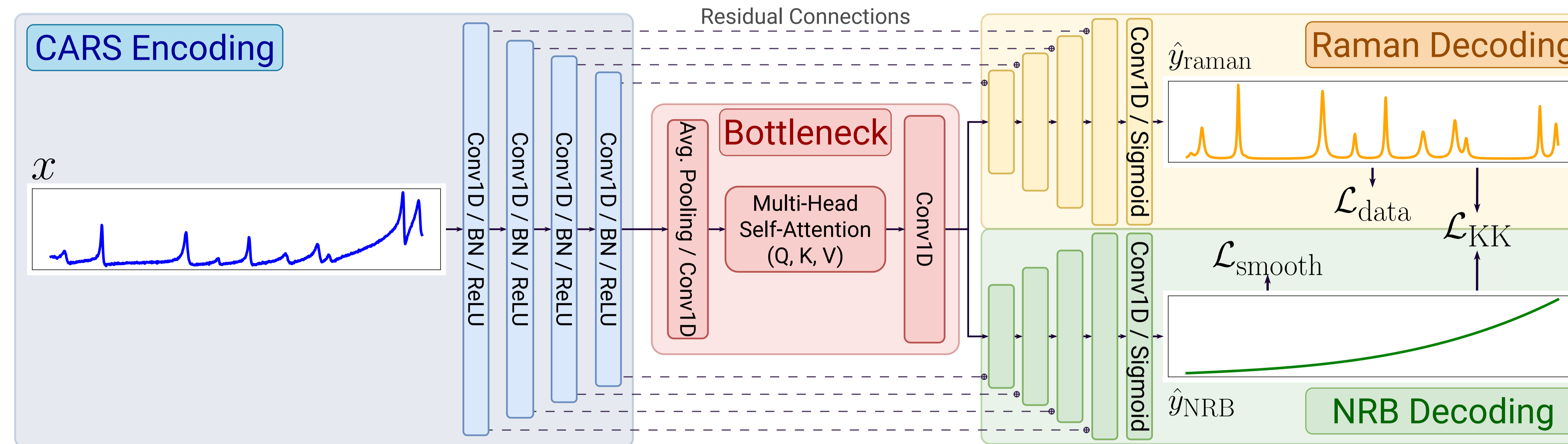
Motivation

- Raman Spectroscopy allows label free molecular analysis but is slower.
- Coherent Anti-Stokes Raman Spectroscopy (CARS) is a faster alternative.
- **Problem:** CARS spectra have dominant Non-Resonant Background (NRB).



Robust, Accurate Raman Signal Extraction

Utilizing Spectroscopic principles in training Neural Networks



Physics-Informed Losses

• **Idea:** Utilize the knowledge from Spectroscopy using Physics-Informed principles to train robust and accurate deep learning models.

• In this case:

- Kramers-Kronig relationships between CARS and Raman Spectra gives:

$$\mathcal{L}_{KK} = |\hat{y}_{\text{raman}} - \mathcal{I}(\mathcal{H}(x - \hat{y}_{\text{NRB}}))|^2.$$

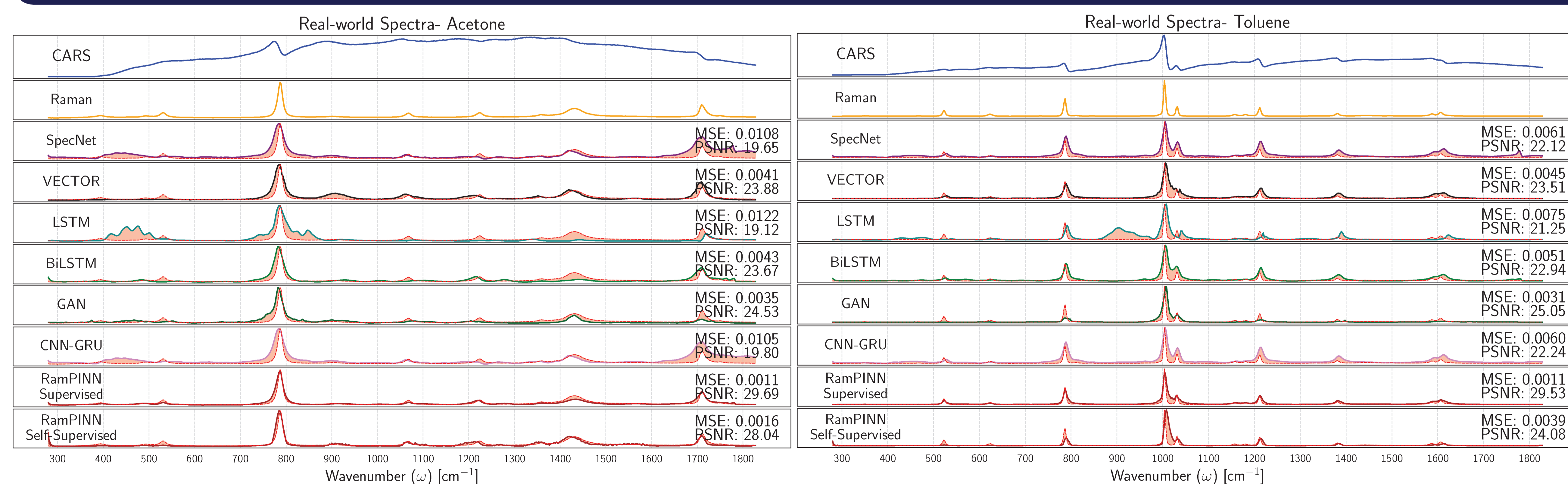
- Non-Resonant Background is smoothly varying:

$$\mathcal{L}_{\text{smooth}} = |\nabla \hat{y}_{\text{NRB}}|^2.$$

- Resulting in our training objective:

$$\mathcal{L}_{\text{total}} = \lambda_{\text{data}} \mathcal{L}_{\text{data}} + \lambda_{\text{KK}} \mathcal{L}_{\text{KK}} + \lambda_{\text{smooth}} \mathcal{L}_{\text{smooth}}$$

Evaluation on Real World Spectra



Results

Method	MSE ↓	PSNR (dB) ↑
TDKK [†]	0.0283	15.48
LeDHT [†]	0.0814	10.91
IWT [†]	0.0139	18.75
SpecNet	0.0064 ± 0.0003	21.91 ± 0.21
VECTOR	0.0205 ± 0.0002	16.88 ± 0.04
LSTM	0.0732 ± 0.1169	19.30 ± 8.77
BiLSTM	0.0007 ± 0.0002	31.57 ± 1.29
GAN	0.0088 ± 0.0118	22.74 ± 3.74
CNN-GRU	0.0019 ± 0.0004	27.38 ± 0.97
RamPINN	0.0006 ± 0.0001	33.83 ± 0.13
RamPINN (Self-sup)	0.0053 ± 0.0003	22.79 ± 0.28

Ablation Studies

